# Argonne Hational Laboratory

MOMENTS OF FIRST-PASSAGE DISTRIBUTIONS
IN SLAB GEOMETRY

by

P. J. Brockwell and J. M. Landwehr

### ARGONNE NATIONAL LABORATORY 9700 South Cass Avenue Argonne, Illinois 60439

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Applied Mathematics Division

December 1968

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#### I. INTRODUCTION

There exists a variety of physical processes having a Markovian character in which a particle suffers a succession of independent collisions with atoms of the medium through which it travels. Examples are the following: the diffuse scattering of light, where the particle is a photon; the diffusion of neutrons; the multiple scattering of charged particles. In connection with such processes, one is often interested in the probability distribution of the state variables of the particles (position, velocity, wavelength, spin, etc.) when they make first passages through some surface in space (regardless of the times of emergence). A general stochastic theory of such first-passage distributions has been developed by Moyal, 10,11 and Brockwell. For a comprehensive account of the theory of branching processes as applied to neutron transport theory, we refer the reader to Mullikin. 13

The following specific transport model will be dealt with in this report. We shall be concerned with a population of particles (for example, neutrons), the state of an individual particle being represented by a vector  $\mathbf{y} = (\mathbf{x}, \boldsymbol{\mu})$ , where  $\mathbf{x}$  denotes position and  $\boldsymbol{\mu}$  denotes direction of motion. (Particle speed is assumed to be essentially constant—this is the classical one-group approximation.) We denote by Y the set of all possible individual states and by  $\mathcal{B}(\mathbf{Y})$  the Borel field of subsets of Y. The population state space Y is then defined by

$$V = \bigcup_{n=0}^{\infty} Y^n,$$

where  $Y^n$ ,  $n \geq 1$ , denotes the n-fold Cartesian product of Y with itself, and  $Y^0$  denotes the state in which the population is empty. Measurable subsets of Y are defined to be those belonging to the  $\sigma$ -field B(Y) generated by the product  $\sigma$ -fields  $B(Y^n)$ ,  $n=0,1,2,\ldots$ . A typical element of Y corresponding to a population of size n will be denoted by  $y^{(n)}$ . (We imagine the particles to be labeled in some way so that  $y^{(n)}$  is an <u>ordered</u> n-tuple.) For a detailed account of the theory of stochastic population processes, see Moyal.

We suppose that the behavior of the population of particles is governed by the following functions (which we assume known from quantum-mechanical or other considerations):

## 1. The total cross section or inverse mean-free-path, $\lambda(\underline{x})$

Given a particle with state  $y=(x,\mu)$ , the probability that it experiences a collision in traveling a small distance  $d\ell$  is  $\lambda(x)d\ell+o(d\ell)$ . The probability of more than one collision in  $d\ell$  is  $o(d\ell)$ .

### 2. The collision outcome distribution, $\{\phi_n\}$

The distribution  $\{\phi_n\}$  is a conditional probability measure on  $\mathcal{B}(y) \times Y$ . More specifically,  $\phi_n(A|y)$  is the probability, given that a particle with state y experiences a collision, that exactly n particles are produced with states  $y_1, \ldots, y_n$  such that  $y(n) = (y_1, \ldots, y_n) \in A$ . Note that the colliding particle itself (if it survives the collision) is included among the particles produced. For photon scattering, where only absorption or scattering are possible,  $\phi_n = 0$  for  $n \geq 2$ . In general,

$$\sum_{n=1}^{\infty} \phi_n(\mathbf{Y}^n|\mathbf{y}) = 1 - \phi_0(\mathbf{y}),$$

where  $\phi_0(y)$  is the probability that the colliding particle is absorbed.

In addition to assuming that  $\lambda$  and  $\{\phi_n\}$  are known, we assume that between collisions each particle experiences a change in position only (i.e.,  $\mu$  is constant). Moreover, we suppose that there is no interaction between the particles themselves, only between the particles and the atoms of the medium through which they move.

The problems we shall discuss here fall into the general class of first-passage problems (see Moyal  $^{10}$ ). Given a single initial particle in a slab of thickness t (infinite in two directions), we specify its position by a single coordinate x ( $0 \le x \le t$ ) and its direction of motion by the cosine  $\mu$  of the angle it makes with the positive x-axis (normal to the slab faces). The problem can be stated as follows: Given a single initial particle with state  $y = (x, \mu)$ , what is the probability distribution of the resulting population of particles making first passages from the slab (the state of each particle in this population being its state as it emerges from the slab)? If the exterior of the slab is vacuous (so that returns to the slab are impossible), then the first-passage population is identical with the total emergent population. We shall use the terms emergent population and first-passage population interchangeably.

For an arbitrary convex body with surface  $\Sigma$ , the number of particles making first passages from the body is a random number n, and the states of the emerging particles can be represented by an element  $y(n) = (y_1, \ldots, y_n)$  of the population state space y. It is useful to introduce the generating functional (conditional on a single initial particle with state y)

$$\begin{split} G(\xi \,|\, \chi) \; &= \; \mathrm{E}\, \xi(y_1) \, \xi(\underline{y}_2) \; \ldots \; \xi(\underline{y}_n) \\ \\ &\equiv \; \mathrm{P}_0(\underline{y}) \, + \; \sum_{n=1}^{\infty} \; \int \underbrace{\dots}_{Y^n} \; \int \xi(\underline{y}_1) \; \dots \; \xi(\underline{y}_n) \mathrm{P}_n(\mathrm{d}\underline{y}_1 \; \dots \; \mathrm{d}\underline{y}_n \, \big| \, \underline{y}), \end{split}$$

where  $\xi$  is an arbitrary measurable function on Y such that

$$\sup_{y \in Y} |\xi(y)| \le 1$$

and  $P_n(A|y)$  is the probability, given a single initial particle with state y, that the state  $y^{(n)}$  of the first-passage population satisfies  $y^{(n)} \in A$ . We then obtain the following stochastic form of the Boltzmann equation (see, for example, Moyal, 11 Pál, 14 Bell, 2 and Brockwell 4):

$$[\underbrace{\mu} \cdot \nabla - \lambda(\underline{x})] G(\xi | \underline{y}) = -\lambda(\underline{x}) \left[ \phi_0(\underline{y}) + \sum_{n=1}^{\infty} \int \dots \int_{Y^n} \phi_n(d\underline{y}_1 \dots d\underline{y}_n | \underline{y}) \prod_{i=1}^n G(\xi | \underline{y}_i) \right],$$

with boundary conditions

$$G(\xi \mid y) = \xi(y)$$
 if  $x$  is on the surface  $\Sigma$  and  $\mu$  is directed outwards, (2)

where  $y = (x, \mu)$ .

The generating functional G uniquely determines (see Moyal<sup>9</sup>) a symmetric distribution on the measurable space (V,B(V)), which is just the probability distribution of the first-passage population. However, the equation for G is difficult to solve because of its nonlinearity. Instead, we shall study the associated moment distributions for which the Boltzmann equation is linear.

We shall assume that  $\phi_n$ , n = 1, 2, ..., takes the form

$$\phi_{\mathbf{n}}(\mathrm{d}\mathbf{y}_{1} \, \dots \, \mathrm{d}\mathbf{y}_{\mathbf{n}} | \mathbf{y}) = \prod_{\mathbf{n}} \left[ \prod_{i=1}^{\mathbf{n}} \delta(\mathbf{x}_{i} - \mathbf{x}) \, \phi(\mathrm{d}\mu_{i} | \mu) \, \mathrm{d}\mathbf{x}_{i} \right], \tag{3}$$

where  $\Pi_n$  is the probability that exactly n particles result from the collision,  $\delta$  is the three-dimensional Dirac delta function, and  $\phi(\mathrm{d} \nu | \mu)$  is the probability that a particle produced by the collision has a direction of motion in the element of solid angle  $\mathrm{d} \nu$  about  $\nu$ . In subsequent sections, we will assume that  $\phi(\mathrm{d} \nu | \mu)$  is of the form

$$\phi(\mathbf{d}_{\mathcal{V}}|\mu) = \sigma(\theta) \, \mathbf{d}_{\mathcal{V}},\tag{4}$$

where  $\theta$  is the angle between  $\underline{\mu}$  and  $\underline{\nu}$ , and that the absorption probability  $\phi_0(y)$  is constant (equal to  $\Pi_0$ ).

The analysis will be confined to slab geometry, so that the state y will be represented by a pair of scalars  $(x,\mu)$  and  $\lambda$  will be a function of x only. By a simple scale transformation, we may assume without loss of generality that  $\lambda$  is constant.

In this report, we shall use the discrete approximation method developed by Brockwell<sup>3</sup> to derive the equations giving the first two moments of the joint first-passage distribution for the model described above. That is, equations will be given for the means, variances, and covariances of the numbers of particles emerging with various states from the slab, conditional on a single initial particle in the slab with given initial state. In addition to calculating solutions of these equations, we shall also use them to estimate the critical length of the slab, i.e., the smallest length for which the mean number of emergent particles becomes infinite. (This is one of the many possible definitions of critical length. For a discussion of the relationship between the various definitions, see Moyal<sup>11</sup> and Brockwell and Moyal.<sup>5</sup>)

The discrete approximation we shall use in the analysis is presented in Section  ${\rm II}.$ 

The development of the equations for the first two moments and the solutions of these equations are given in Section III.

A computer program was written to calculate the solutions, and the results are given for a variety of different collision outcome distributions in Section IV. The appendix gives in detail the mathematical methods used in the computer code to solve the equations.

### II. THE BASIS OF THE DISCRETE APPROXIMATION

The icosahedral approximation developed by Brockwell<sup>3</sup> is used. A complete discussion of this approximation is given in Chapter VI of Ref. 3, so only a summary is given here. We are concerned with scattering, absorption, and fission in a plane slab, infinite in two directions and with finite thickness t.

(5)

The state of any particle is determined by its position and direction of motion. (We consider only the case of particles with a single energy, i.e., the one-group case, although there is no conceptual difficulty in the generalization involving multiple energies. In fact, H. Greenspan (of the ANL Applied Mathematics Division) is currently working on a computer program using analogs of the equations developed in Section III for particles with a finite set of possible energies. His results will provide the first- and second-moment structure for the more realistic case in which the dependence of  $\lambda$  and  $\{\phi_n\}$  on energy, or other additional state variables, is taken into account.) The position of any particle is specified by its distance x  $(0 \le x \le t)$  from the left face of the slab. It is in the specification of the direction of motion that the icosahedral approximation enters.

The essential approximation to the model described in Section I is the following: The directions of motion of each particle are constrained to a set of 30 unit vectors corresponding to points evenly spaced on the surface of the unit sphere. That is, a particle may not travel in an arbitrary direction, but only in directions represented by these 30 unit vectors.

The 30 vectors are chosen in the following way: A regular icosahedron is oriented as in Fig. 1 so that the line joining its center to the midpoint of one edge is in the direction of the unit vector  $\underline{i}$  normal to the



Fig. 1. Orientation of the Icosahedron

slab faces (and in the direction of increasing x). The 30 possible directions of motion are then taken to be along the lines joining the center of the icosahedron to the midpoints of its edges. If we let  $\{\underline{a}_1, \ldots, \underline{a}_{30}\}$  be the unit vectors in these directions, then the set of scalar products  $\{\underline{a}_1 \cdot \underline{a}_1, \underline{a}_1 \cdot \underline{a}_2, \ldots, \underline{a}_1 \cdot \underline{a}_{30}\}$  gives the cosines of the possible angular deflections for a particle initially traveling in direction  $\underline{a}_i$ . This (unordered)

set is the same for each i ( $i=1,\ldots,30$ ). This means that for any direction of motion before a collision, the set of all possible angular deflections resulting from the collision is the same, independent of the initial direction of motion; that is, we can define a single set of 30 possible angular deflections  $\{\epsilon_1,\ldots,\epsilon_{30}\}$  which take an arbitrary initial direction  $a_i$  into the set  $\{a_1,\ldots,a_{30}\}$  of all possible directions of motion. This set  $\{\epsilon_1,\ldots,\epsilon_{30}\}$  contains only nine distinct angles  $\theta_1,\ldots,\theta_9$ , where

$$\cos \theta_1 = \mu_1,$$
  $\cos \theta_9 = -\mu_1,$   
 $\cos \theta_2 = \mu_2,$   $\cos \theta_8 = -\mu_2,$   
 $\cos \theta_3 = \mu_3,$   $\cos \theta_7 = -\mu_3,$   
 $\cos \theta_4 = \mu_4,$   $\cos \theta_6 = -\mu_4,$   
 $\cos \theta_5 = \mu_5,$ 

and

$$\mu_{1} = 1 = -\mu_{10},$$

$$\mu_{2} = \frac{1}{4} (1 + \sqrt{5}) = -\mu_{9},$$

$$\mu_{3} = \frac{1}{2} = -\mu_{8},$$

$$\mu_{4} = \frac{1}{4} (\sqrt{5} - 1) = -\mu_{7},$$

$$\mu_{5} = 0 = -\mu_{6}.$$
(6)

With the orientation of the icosahedron defined above, the cosines of the angles between the 30 vectors representing possible directions of motion and the positive x-axis take only nine distinct values,  $\mu_1, \ldots, \mu_5$  (= $\mu_6$ ),  $\mu_7, \ldots, \mu_{10}$ , where the  $\mu_i$ 's are defined in Eq. 6. Considerable simplification can therefore be achieved by grouping the directions of motion according to the cosine of the angle they make with the positive x-axis. The number  $\alpha(\alpha=1,\ldots,10)$  will be used to denote the set of all directions of motion whose direction cosine is  $\mu_{\alpha}$ . The definition must be modified slightly for the directions 5 and 6 perpendicular to the x-axis. Direction 5 consists (see Fig. 1) of the two unit vectors  $\pm k$ , and direction 6 consists of the unit vectors  $\pm j$ . This splitting of the directions perpendicular to the x-axis is necessary so that the process, when defined in terms of the state variables  $(x,\alpha)$ , be Markovian. We say that a particle has state  $(x,\alpha)$  if its distance from the left end of the slab is  $x(0 \le x \le t)$ , and the cosine of its direction of motion is  $\mu_{\alpha}$  ( $\alpha=1,\ldots,10$ ).

In practice, of course, the particle can move in any direction in space. When a particle makes a collision with an atom of the slab, it gives rise to a random number (n = 0, 1, 2, ...) of particles of the same type. As described in Eq. 3, we shall assume that, conditional on a particle with direction  $\underline{\mu}$  experiencing a collision and giving rise to n particles (n  $\geq$  1), the directions of motion of the resulting particles are independently and identically distributed with distribution  $\phi(d\,\underline{\nu}\,|\,\mu)$ , where

$$\phi(\mathbf{d}\chi|\mu) = \sigma(\theta)\,\mathbf{d}\chi,\tag{7}$$

 $\theta$  is the angle between  $\underline{\nu}$  and  $\underline{\mu}$ , and  $d\underline{\nu}$  is an element of solid angle surrounding the unit vector  $\underline{\nu}$ . We must determine  $p_1, \ldots, p_9$  corresponding to the continuous function  $\sigma(\theta)$ . Since the original vectors  $\{\underline{a}_1, \ldots, \underline{a}_{30}\}$  each

correspond to congruent regions of the unit sphere, the probabilities are chosen so that

$$p_i = k\sigma(\theta_i), \quad i = 1, ..., 9, \tag{8}$$

the constant k being determined by the normalization condition,

$$p_1 + 4 \sum_{i=2}^{8} p_i + p_9 = 1.$$
 (9)

For example, if scattering is isotropic, then  $\sigma(\theta) = 1/(4\pi)$ , and Eqs. 8 and 9 give

$$p_1 = p_2 = \dots = p_9 = \frac{1}{30}.$$

If a particle with direction of motion  $i\ (i=1,\ ...,\ 10)$  makes a collision that results in the production of n particles  $(n\ge 1)$ , then the directions of motion of the resulting particles are independently distributed, the distribution depending on the direction of motion of the colliding particle. This common distribution is specified (in the discrete model) by the probabilities

P<sub>ij</sub> = Prob {the resulting particle emerges from the collision with direction j, given that the colliding particle was traveling in direction i just before the collision}.

These probabilities must satisfy the normalization condition,

$$\sum_{j=1}^{10} P_{ij} = 1, \quad i = 1, ..., 10.$$
 (10)

The probabilities  $P_{ij}$  depend on which of the angular deflections  $\theta_1, \ldots, \theta_9$  can bring about a transition from direction i to direction j, and this in turn depends on the geometry of the icosahedron. For example, a transition from direction 2 to direction 2 can occur by deflections through  $\theta_1, \theta_2, \theta_3$ , or  $\theta_4$ , and consequently  $P_{22} = p_1 + p_2 + p_3 + p_4$ . The other  $P_{ij}$ 's are found similarly and are shown below as the matrix P in which  $P_{ij}$  is the jth element of the ith row and the symbol  $(i_1, i_2, \ldots, i_n)$  is used as an abbreviation for  $p_{i_1} + \ldots + p_{i_n}$ .

$$P = \begin{bmatrix} (1) & (2222) & (3333) & (4444) & (55) & (55) & (6666) & (7777) & (8888) & (9) \\ (2) & (1234) & (2345) & (2356) & (46) & (37) & (4578) & (5678) & (6789) & (8) \\ (3) & (2345) & (1267) & (2457) & (28) & (46) & (3568) & (3489) & (5678) & (7) \\ (4) & (2356) & (2457) & (1368) & (37) & (28) & (2479) & (3568) & (4578) & (6) \\ (5) & (4466) & (2288) & (3377) & (19) & (55) & (3377) & (2288) & (4466) & (5) \\ (5) & (3377) & (4466) & (2288) & (55) & (19) & (2288) & (4466) & (3377) & (5) \\ (6) & (4578) & (3568) & (2479) & (37) & (28) & (1368) & (2457) & (2356) & (4) \\ (7) & (5678) & (3489) & (3568) & (28) & (46) & (2457) & (1267) & (2345) & (3) \\ (8) & (6789) & (5678) & (4578) & (46) & (37) & (2356) & (2345) & (1234) & (2) \\ (9) & (8888) & (7777) & (6666) & (55) & (55) & (4444) & (3333) & (2222) & (1) \end{bmatrix}$$

Note that each row contains  $p_1$  and  $p_9$  once and each of  $p_2, \ldots, p_8$  four times. This is because each probability  $p_1$  corresponds to a particular <u>unit vector</u> representing the direction of motion of the particle after the collision, and, of the 30 possible unit vectors, exactly four correspond to each angular deflection  $\theta_2, \ldots, \theta_8$ . Thus Condition 9 implies Condition 10.

### III. EQUATIONS FOR FIRST AND SECOND MOMENTS

In this section we develop the equations for the mean number of particles emerging in direction  $\alpha$   $(\alpha=1,\,...,\,4,\,7,\,...,\,10)$  conditional on an initial particle at position x  $(0\leq x\leq t)$  within the slab and traveling in direction  $\beta$   $(\beta=1,\,...,\,10).$  Particles cannot emerge traveling in direction 5 or 6, as these directions are parallel to the faces of the slab. The equations are also derived giving the variance-covariance structure of the number of particles emergent in direction  $\alpha_1$  and  $\alpha_2$   $(\alpha_1=1,\,...,\,4,\,7,\,...,\,10)$ ;  $\alpha_2=1,\,...,\,4,\,7,\,...,\,10)$  conditional on a particle at position x  $(0\leq x\leq t)$  and traveling in direction  $\beta$   $(\beta=1,\,...,\,10).$  The solutions of these equations are then presented.

Denote by  $N = (N_1, \ldots, N_4, N_7, \ldots, N_{10})$  the numbers of particles making first passages from the slab  $0 \le x \le t$  in directions  $1, \ldots, 4, 7, \ldots, 10$ , respectively, and let  $P(N \mid x, \nu)$  be the probability that N particles make first passages from the slab conditional on a single initial particle with position x and direction cosine  $\nu$ . Similarly, let  $P(N \mid x, \nu_1, \ldots, \nu_k)$  denote the probability that N particles make first passages conditional on N initial particles with position N and direction cosines N, ..., N (-1  $\le \nu_1 \le 1$ , N). It is convenient to introduce the generating functions

$$G(\mathbf{x}, \nu) = \sum_{n_1, \dots, n_4, n_7, \dots, n_{10} = 0}^{\infty} P(\underline{\mathbf{n}} | \mathbf{x}, \nu) z_1^{n_1} \dots z_4^{n_4} z_7^{n_7} \dots z_{10}^{n_{10}}, |z_{\mathbf{i}}| \le 1,$$

and

$$G(\mathbf{x},\nu_1,\;\ldots,\nu_k) \; = \; \sum_{n_1,\ldots,n_4,n_7,\ldots,n_{10}=0}^{\infty} \; \mathbb{P}\left(\underline{n}\;\big|\,\mathbf{x},\nu_1,\ldots,\nu_k\right) z_1^{n_1}\ldots z_4^{n_4} z_7^{n_7}\ldots z_{10}^{n_{10}},\;\big|\,z_{\hat{1}}\,\big| \leq 1.$$

For clarity in writing G, we will suppress the arguments  $\mathbf{z}_i$ . Then, since we are assuming that the particles do not interact with each other,

$$G(x, \nu_1, ..., \nu_k) = G(x, \nu_1) ... G(x, \nu_k).$$

The probability that a particle makes a collision in traveling a small distance  $\delta s$  is assumed to be  $\lambda \delta s + o(\delta s)$ , where  $\lambda$  is a positive constant. The probability of more than one collision is  $o(\delta x)$ . By measuring all distances in units of  $\lambda^{-1}$ , we can assume (without loss of generality) that  $\lambda = 1$ .

Given that a particle moving with direction cosine  $\nu$  experiences a collision, we assume that there is a probability  $\pi_0$  that the particle is absorbed and probabilities  $\pi_k(\mathrm{d}\nu_1,\,\ldots,\,\mathrm{d}\nu_k\,|\,\nu),\,\,k=1,\,2,\,\ldots,$  that k particles are produced with direction cosines in  $\mathrm{d}\nu_1,\,\ldots,\,\mathrm{d}\nu_k$  (-1  $\leq$   $\nu_1$   $\leq$  1). In the discrete model,  $\nu_1$  will take one of the values  $\mu_{\alpha},\,\alpha=1,\,\ldots,\,10$ , with probability 1.

The initial particle will either experience no collisions before leaving the slab (in which case exactly one particle will emerge from the slab with direction cosine  $\nu$ , or the particle will experience a first collision at some point y within the slab. By considering these two possibilities, we obtain the first collision equation for  $G(x, \nu)$ :

$$\begin{split} G(\mathbf{x},\nu) &= e^{-\nu^{-1}\left(t-\mathbf{x}\right)} \prod_{\alpha=1,\ldots,4,7,\ldots,10} z_{\alpha}^{\delta\,\nu\,\cdot\mu\alpha} + \int_{y=\mathbf{x}}^{t} \pi_0 e^{-\nu^{-1}\left(y-\mathbf{x}\right)} \nu^{-1} \,\mathrm{d}y \\ &+ \sum_{k=1}^{\infty} \int_{y=\mathbf{x}}^{t} \int_{-1}^{1} \ldots \int_{-1}^{1} \pi_k (\mathrm{d}\nu_1,\,\ldots,\,\mathrm{d}\nu_k|\nu) G(y,\nu_1) \ldots G(y,\nu_k) e^{-\nu^{-1}\left(y-\mathbf{x}\right)} \nu^{-1} \,\mathrm{d}y, \quad \text{if } \nu > 0\,, \end{split}$$

$$G(\mathbf{x}, \nu) = e^{\nu^{-1}\mathbf{x}} \prod_{\alpha=1,...,4,7,...,10} z_{\alpha}^{\delta_{\nu},\mu_{\alpha}} + \int_{y=0}^{x} \pi_{0}e^{-\nu^{-1}(y-\mathbf{x})_{\nu^{-1}}} dy$$

$$+ \sum_{k=0}^{\infty} \int_{y=0}^{x} \int_{-1}^{1} ... \int_{-1}^{1} \pi_{k}(d\nu_{1}, ..., d\nu_{k}|\nu)G(y,\nu_{1})...G(y,\nu_{k})e^{-\nu^{-1}(y-\mathbf{x})_{\nu^{-1}}} dy, \quad \text{if } \nu < 0. \quad (13)$$

 $(\delta_{\nu,\mu}$  is defined to be one if  $\nu=\mu$ , zero otherwise.) Differentiating Eqs. 12 and 13 with respect to x, we obtain the "backward" Kolmogorov equation,

$$\nu \frac{\partial}{\partial \mathbf{x}} G(\mathbf{x}, \nu) - G(\mathbf{x}, \nu) = -\pi_0 - \sum_{k=1}^{\infty} \int_{-1}^{1} ... \int_{-1}^{1} \pi_k (\mathrm{d}\nu_1 ... \mathrm{d}\nu_k \big| \nu) G(\mathbf{x}, \nu_1) ... G(\mathbf{x}, \nu_k), \tag{14}$$

with boundary conditions

$$G(\mathbf{x}, \nu) = \prod_{\alpha=1,\dots,4,7,\dots,10} \mathbf{z}_{\alpha}^{\delta_{\nu}, \mu\alpha} \quad \text{if } \mathbf{x} = 0 \text{ and } \nu < 0, \\ \text{or } \mathbf{x} = \mathbf{t} \text{ and } \nu > 0.$$
 (15)

(These equations are in fact a special case of Eqs. 1 and 2.)

We now make the further assumption (in accordance with Eq. 3) that the probability measures  $\pi_k$ ,  $k \ge 1$ , have the form

$$\pi_{\mathbf{k}}(\mathrm{d}\nu_{1},\ldots,\mathrm{d}\nu_{\mathbf{k}}|\nu) = \pi_{\mathbf{k}}\pi(\mathrm{d}\nu_{1}|\nu)\pi(\mathrm{d}\nu_{2}|\nu)\ldots\pi(\mathrm{d}\nu_{\mathbf{k}}|\nu), \tag{16}$$

where  $\pi_k$  is the probability that k particles are produced and

$$\int_{-1}^{1} \pi(\mathrm{d}\nu_{\mathbf{i}}|\nu) = 1.$$

The backward equation then becomes

$$\left[\mu \frac{\partial}{\partial \mathbf{x}} - 1\right] G(\mathbf{x}, \mu) = -\pi_0 - \sum_{k=1}^{\infty} \pi_k \left[ \int_{-1}^{1} \pi(\mathrm{d}\nu | \mu) G(\mathbf{x}, \nu) \right]^k, \tag{17}$$

with the same boundary conditions as above.

Let  $M_{\alpha}(x,\mu)$  denote the expected number of particles emerging from the slab with direction  $\alpha$  (i.e., with direction cosine  $\mu_{\alpha}$ ),  $\alpha$  = 1, ..., 4, 7, ..., 10. Then, under the assumption that  $M_{\alpha}$  is bounded and

$$\sum_{0}^{\infty} k \pi_{k} = m < \infty,$$

we have

$$M_{\alpha}(\mathbf{x}, \mu) = \left[\frac{\partial}{\partial \mathbf{z}_{\alpha}} G(\mathbf{x}, \mu)\right]_{\mathbf{z}_{\beta}=1, \beta=1, \dots, 4, 7, \dots, 10}.$$
 (18)

Hence, from Eqs. 17 and 15,

$$\left[\mu \frac{\partial}{\partial \mathbf{x}} - 1\right] \mathbf{M}_{\alpha}(\mathbf{x}, \mu) = -\mathbf{m} \int_{-1}^{1} \pi(\mathrm{d}\nu | \mu) \mathbf{M}_{\alpha}(\mathbf{x}, \nu), \tag{19}$$

and

$$M_{\alpha}(\mathbf{x}, \mu) = \delta_{\mu, \mu_{\alpha}}$$
 if  $\mathbf{x} = 0$  and  $\mu < 0$ ,  
or  $\mathbf{x} = t$  and  $\mu > 0$ . (20)

(In deriving Eq. 19 from Eqs. 17 and 18, we have used the fact that

$$[G(\mathbf{x}, \mu)]_{\mathbf{z}_{\beta}=1, \beta=1, \dots, 4, 7, \dots, 10} = 1.$$

This follows from our assumption that  $M_{\alpha}$  is bounded.)

The second factorial moments of the numbers of emergent particles are obtained by a further differentiation of the generating function G. Thus, if we define

$$\mathbf{S}_{\alpha\beta}(\mathbf{x},\mu) = \begin{cases} \mathbf{E}\mathbf{N}_{\alpha}\mathbf{N}_{\beta} & \alpha \neq \beta \\ \mathbf{E}[\mathbf{N}_{\alpha}(\mathbf{N}_{\alpha}-1)] & \beta = \alpha \end{cases}$$

(assuming again that these moments are bounded), then

$$S_{\alpha\beta}(\mathbf{x},\mu) = \left[\frac{\partial^2}{\partial z_{\alpha}\partial z_{\beta}} G(\mathbf{x},\mu)\right]_{z_1 = \dots = z_4 = z_7 = \dots = z_{10} = 1}.$$
 (21)

Provided

$$\sum_{k=0}^{\infty} \; k(k\text{-}1)\pi_k \; = \; m_{\left(2\right)} < \infty, \label{eq:mass_problem}$$

we then have, from Eqs. 15, 17, and 21,

$$\left[\mu \frac{\partial}{\partial \mathbf{x}} - 1\right] S_{\alpha\beta}(\mathbf{x}, \mu) = -m \int_{-1}^{1} \pi(\mathrm{d}\nu | \mu) S_{\alpha\beta}(\mathbf{x}, \nu)$$

$$-m_{(2)} \left\{ \int_{-1}^{1} \pi(\mathrm{d}\nu | \mu) M_{\alpha}(\mathbf{x}, \nu) \right\} \left\{ \int_{-1}^{1} \pi(\mathrm{d}\nu | \mu) M_{\beta}(\mathbf{x}, \nu) \right\}.$$
(22)

and

$$S_{\alpha\beta}(\mathbf{x},\mu) = 0$$
 if  $\mathbf{x} = 0$  and  $\mu < 0$ ,  
or  $\mathbf{x} = t$  and  $\mu > 0$ . (23)

(Equations 22 and 23 are valid whether or not  $\alpha = \beta$ .)

So far we have not fully exploited our discrete approximation in deriving the equations for  $M_{\alpha}$  and  $S_{\alpha}{}_{\beta}.$  In the discrete approximation, the initial direction  $\mu$  can take only one of the values  $\{\mu_1,\ldots,\mu_{10}\}$  defined in Section II, and the integrals with respect to the measure  $\pi$  are in fact sums. Thus,

$$\int_{-1}^{1} M_{\alpha}(\mathbf{x}, \nu) \pi(d\nu | \mu_{\mathbf{i}}) = \sum_{j=1}^{10} M_{\alpha}(\mathbf{x}, \mu_{\mathbf{j}}) P_{\mathbf{i}\mathbf{j}},$$

where  $P_{ij}$  is the probability that a particle produced at a collision travels in direction j conditional on the colliding particle traveling in direction i before the collision. Thus  $P_{ij}$  is the (i,j)th element of the matrix given in Eq. 11. Similarly,

$$\int_{-1}^{1} S_{\alpha\beta}(\mathbf{x}, \nu) \pi(\mathrm{d}\nu | \mu_{\mathbf{i}}) = \sum_{j=1}^{10} S_{\alpha\beta}(\mathbf{x}, \mu_{\mathbf{j}}) P_{\mathbf{i}\mathbf{j}}.$$

It is now convenient to change notation slightly. We write  $M_{\alpha}(\mathbf{x},i)$  for  $M_{\alpha}(\mathbf{x},\mu_i)$  (i = 1, ..., 10). Thus  $M_{\alpha}(\mathbf{x},i)$  is the mean number of particles emergent in direction  $\alpha$  ( $\alpha$  = 1, ..., 4, 7, ..., 10), conditional on one particle at position  $\mathbf{x}$  ( $0 \le \mathbf{x} \le t$ ) traveling in direction i. The cosine of the angle between the direction of motion i and the positive x-axis is therefore  $\mu_i$ . Similarly, we write  $S_{\alpha}\beta(\mathbf{x},i)$  for  $S_{\alpha}\beta(\mathbf{x},\mu_i)$  (i = 1, ..., 10). Thus Eq. 19 may be written in matrix form,

$$\begin{bmatrix} \mu_{1} \frac{\partial}{\partial x} - 1 & 0 \\ \vdots \\ 0 & \mu_{10} \frac{\partial}{\partial x} - 1 \end{bmatrix} \begin{bmatrix} M_{\alpha}(x, 1) \\ \vdots \\ M_{\alpha}(x, 10) \end{bmatrix} = -m \begin{bmatrix} P_{1 \ 1} \dots P_{1 \ 10} \\ \vdots \\ P_{10 \ 1} & P_{10 \ 10} \end{bmatrix} \cdot \begin{bmatrix} M_{\alpha}(x, 1) \\ \vdots \\ M_{\alpha}(x, 10) \end{bmatrix}.$$
(24)

Since  $\mu_5 = \mu_6 = 0$ , we can write  $M_{\alpha}(x,5)$  and  $M_{\alpha}(x,6)$  as linear functions of  $M_{\alpha}(x,1)$ , ...,  $M_{\alpha}(x,4)$ ,  $M_{\alpha}(x,7)$ , ...,  $M_{\alpha}(x,10)$ . Doing this, and rearranging the terms, we may express Eq. 24 as

$$\frac{\partial}{\partial \mathbf{x}} \begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 4) \\ \mathbf{M}_{\alpha}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix} = \mathbf{R} \begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 4) \\ \mathbf{M}_{\alpha}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix}, \tag{25}$$

where R is an  $8 \times 8$  matrix which can be determined from Eq. 24. This is a system of eight homogeneous first-order linear differential equations, with boundary conditions given by Eq. 20. The solution is

$$\begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 4) \\ \mathbf{M}_{\alpha}(\mathbf{x}, 7) \\ \vdots \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix} = e^{\mathbf{R}\mathbf{X}} \cdot \mathbf{g}, \tag{26}$$

where exp(Rx) is the 8 x 8 matrix defined as

$$\sum_{k=0}^{\infty} (Rx)^k / k!,$$

and  $\underline{c}$  is an eight-component column vector determined by the boundary conditions.

In fact, if we let M(x) be the 8 x 8 matrix

$$\begin{bmatrix} M_{1}(x,1) & \dots & M_{4}(x,1)M_{7}(x,1) & \dots & M_{10}(x,1) \\ \vdots & & & \vdots \\ M_{1}(x,4) & \dots & M_{4}(x,4)M_{7}(x,4) & \dots & M_{10}(x,4) \\ M_{1}(x,7) & \dots & M_{4}(x,7)M_{7}(x,7) & \dots & M_{10}(x,7) \\ \vdots & & & \vdots \\ M_{1}(x,10) & \dots & M_{4}(x,10)M_{7}(x,10) & \dots & M_{10}(x,10) \end{bmatrix},$$

$$(27)$$

then

$$M(x) = e^{Rx} \cdot C, \tag{28}$$

where C is an 8 x 8 matrix determined by the boundary conditions. Using the boundary conditions for x = 0 to get the lower half of C, and for x = t to get the upper half of M(t), we have (by matrix partitioning)

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{A} & \mathbf{B} \end{bmatrix} = \begin{bmatrix} \mathbf{E}_{11} & \mathbf{E}_{12} \\ \mathbf{E}_{21} & \mathbf{E}_{22} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{C}_1 & \mathbf{C}_2 \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \tag{29}$$

where

$$\begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} = \exp(Rt),$$

and each of the indicated smaller matrices above is  $4 \times 4$ . Thus,  $C_1 = E_{11}^{-1}$  and  $C_2 = -E_{11}^{-1} \cdot E_{12}$ . Since  $M_{\alpha}(x,5)$  and  $M_{\alpha}(x,6)$  ( $\alpha=1,\ldots,4,7,\ldots,10$ ) can be expressed as linear functions of the terms in M(x), the above gives a complete solution for the mean number of particles emergent in any of the eight possible emergent directions, conditional on one particle at an arbitrary position x within the slab, traveling in any of the 10 possible directions.

The above equations implicitly assume that the mean number of particles produced is finite. If the slab is supercritical, i.e., if the length of the slab is such that the mean of the total number of particles produced is infinite, then these equations will not be valid. However, this method may be used to determine the critical length for a given m

$$\left(=\sum_{k=0}^{\infty}k\pi_{k}\right)$$

by varying the length t of the slab, and seeing for which value of t the total mean number of particles produced approaches infinity. This has been done, and the results are reported in Section IV.

To find the functions  $S_{\alpha,\beta}$ , we now apply similar methods to those used above. Employing the relationship between  $\pi(\mathrm{d}\nu\,|\,\mu)$  and the matrix P, we may write Eq. 22 as

$$\begin{bmatrix} \mu_1 \frac{\partial}{\partial \mathbf{x}} - 1 & 0 \\ & \ddots & \\ & & \ddots & \\ & & & \mu_{10} \frac{\partial}{\partial \mathbf{x}} - 1 \end{bmatrix} \begin{bmatrix} \mathbf{S}_{\alpha\beta}(\mathbf{x}, 1) \\ & &$$

$$-\mathbf{m}_{(2)}\begin{bmatrix} \mathbf{F}_{\alpha\beta}(\mathbf{x},1) \\ \vdots \\ \mathbf{F}_{\alpha\beta}(\mathbf{x},10) \end{bmatrix} \qquad (\alpha = 1, ..., 4, 7, ..., 10; \beta = 1, ..., 4, 7, ..., 10),$$
(30)

$$\text{where } \mathbf{F}_{\alpha\,\beta}(\mathbf{x},\mathbf{i}) = \left\{ \sum_{j=1}^{10} \, \mathbf{M}_{\alpha}(\mathbf{x},j) \mathbf{P}_{ij} \right\} \cdot \left\{ \sum_{j=1}^{10} \, \mathbf{M}_{\beta}(\mathbf{x},j) \cdot \mathbf{P}_{ij} \right\} \quad (i=1,\ldots,10).$$

But, since  $\mu_5 = \mu_6 = 0$ , we can again write  $S_{\alpha\beta}(x,5)$  and  $S_{\alpha\beta}(x,6)$  as linear functions of  $S_{\alpha\beta}(x,i)$  (i = 1, ..., 4, 7, ..., 10) and  $F_{\alpha\beta}(x,i)$  (i = 5,6). Then,

$$\frac{\partial}{\partial \mathbf{x}} \begin{bmatrix} \mathbf{S}_{\alpha \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 4) \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 10) \end{bmatrix} = \mathbf{R} \begin{bmatrix} \mathbf{S}_{\alpha \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 4) \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 10) \end{bmatrix} + \begin{bmatrix} \mathbf{V}_{\alpha \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{V}_{\alpha \beta}(\mathbf{x}, 4) \\ \mathbf{V}_{\alpha \beta}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{V}_{\alpha \beta}(\mathbf{x}, 7) \end{bmatrix}, \tag{31}$$

where R is the same 8 x 8 matrix that appeared in Eq. 25, and  $V_{\alpha}\beta(x,i)$  incorporates  $m_{(2)}$  and is a linear function of  $F_{\alpha}\beta(x,i)$ ,  $F_{\alpha}\beta(x,5)$ , and  $F_{\alpha}\beta(x,6)$  (i = 1,...,4,7,...,10).

Here we have a set of eight first-order, linear, nonhomogeneous differential equations. The solution is analogous to the solution of a first-order, linear, nonhomogeneous differential equation,

$$\begin{bmatrix} S_{\alpha\beta}(\mathbf{x}, 1) \\ \vdots \\ S_{\alpha\beta}(\mathbf{x}, 4) \\ S_{\alpha\beta}(\mathbf{x}, 7) \\ \vdots \\ S_{\alpha\beta}(\mathbf{x}, 10) \end{bmatrix} = e^{\mathbf{R}\mathbf{x}} \cdot \mathbf{c} + \int_{0}^{\mathbf{x}} e^{\mathbf{R}(\mathbf{x} - \mathbf{y})} \cdot \mathbf{v}_{\alpha\beta}(\mathbf{y}) \, d\mathbf{y}, \tag{32}$$

where  $V_{\alpha\beta}(y)$  is the eight-component vector given in Eq. 31. The eight-component vector  $\underline{c}$  is determined by the boundary conditions in Eq. 23. In fact, since  $S_{\alpha\beta}(0) = \underline{c}$ , the bottom four elements of  $\underline{c}$  are zeros. The top four elements are determined using the fact that the top four elements of  $S_{\alpha\beta}(t)$  are zeros.

The covariances, variances, and correlations can then be calculated from the  $S_{\alpha\,\beta}$ 's and the  $M_{\alpha}$ 's by the appropriate formulas. The appendix gives the mathematical methods and details used in writing the computer program that determines the  $M_{\alpha}$ 's and the  $S_{\alpha\,\beta}$ 's.

#### IV. NUMERICAL RESULTS

The numerical results concerning the first- and second-moment structure of the first-passage distribution are presented in this section. First, however, is a discussion of the accuracy of the approximate model used, and of the methods used to verify that the program was coded correctly.

This model does not permit particles to take arbitrary directions of motion within the slab; only the 30 directions corresponding to the midpoints of the edges of an icosahedron are permitted. The question of the accuracy of results from this model, relative both to exact results and to results from models using different approximations, is discussed by Brockwell, Chapter VII, Sections 5 and 6. For problems in slab geometry involving only scattering and absorption, exact solutions are possible in terms of the X- and Y-functions of Chandrasekhar. Numerical comparisons given in Ref. 3 show that the icosahedral approximation compares favorably with the Gaussian quadrature approximation with n=4 and the spherical harmonics method with n=3. This suggests that the icosahedral approximation should give accurate results for other cases in which the exact solutions are not known.

Internal symmetries in the model were used to verify that the coding was done correctly, that is, that the numerical output corresponds to the mathematical analysis. Considering the symmetry inherent in our model, we see that  $M_{\alpha}(x,\ell) = M_{11-\alpha}(t-x,11-\ell)$  ( $0 \le x \le t$ ;  $\alpha=1,\ldots,4,7,\ldots,10$ ;  $\ell=1,\ldots,10$ ). The output for the  $M_{\alpha}$ 's conditional on a particle at position x was compared with the output conditional on a particle at position t-x ( $0 \le x \le t$ ), and it was verified that the required symmetries did in fact hold for the numerical output. Similarly,  $S_{\alpha\beta}(x,\ell) = S_{\beta\alpha}(x,\ell)$ , and  $S_{\alpha\beta}(x,\ell) = S_{11-\alpha,11-\beta}(t-x,11-\ell)$  ( $\alpha=1,\ldots,4,7,\ldots,10$ ;  $\beta=1,\ldots,4,7,\ldots,10$ ;  $0 \le x \le t$ ;  $\ell=1,\ldots,10$ ). The  $S_{\alpha\beta}(x,\ell)$ 's were calculated for  $\alpha=1,\ldots,4$ ;  $\beta=1,\ldots,4,7,\ldots,10$ ; and  $\ell=1,\ldots,4,7,\ldots,10$ . The required symmetries were again satisfied by the numerical output.

### A. Calculations of the Critical Length

We shall take the critical length to of a slab to be the smallest length for which the mean Eqs. 19 and 20 have no bounded nonnegative solution; tc depends on m, the mean number of particles produced per collision, and also upon the scattering law  $\sigma(\theta)$ . (We have assumed this applies to fission products as well as to truly scattered particles; it would not be difficult to extend our method to the case where one angular distribution applies to scattered particles and another to fission-produced particles.) Now, as we increase the slab thickness (starting from t = 0), the mean number of emergent particles mtot (conditional on a single initial particle incident normally upon the slab) increases, approaching ∞ as t † tc. If t is increased slightly beyond tc, the mean numbers of emergent particles in some directions (as calculated from Eqs. 19 and 20 become negative. Since the difference between the smallest t giving negative means and the largest t for which we can find large positive solutions of Eqs. 19 and 20 is small, we can estimate to fairly accurately (within the limits of the icosahedral model) from the numerical results. This was done for two scattering laws-isotropic scattering and Rayleigh scattering (the latter being used primarily to give an idea of the sensitivity of the results to deviations from isotropy).

For isotropic scattering,  $\sigma(\theta)=1/(4\pi)$ ; therefore the directions of motion immediately after a collision are uniformly distributed over the unit sphere, and independent of the direction of motion immediately before the collision. This scattering law is often used as a reasonable approximation for neutron multiplication. For Rayleigh scattering,  $\sigma(\theta)=3(1+\cos^2\theta)/(16\pi)$ . With this scattering law, particles emerging from a collision are more likely to move in a forward or backward direction than perpendicular to the direction of motion of the colliding particle. The Rayleigh scattering law is often used when studying the passage of photons through stellar atmospheres. Other scattering laws relevant to different physical situations can be analyzed without essential modification of the computer program.

Table I gives the critical length  $t_{\rm C}$  for several values of m for both isotropic and Rayleigh scattering. The distance  $t_{\rm C}$  is measured in units of the mean free path  $1/\lambda$ . No method is known that will give the exact value of  $t_{\rm C}$  for either isotropic or Rayleigh scattering. (The method of Case<sup>6</sup> can in principle be used to give any required degree of accuracy, but the analysis becomes extremely complicated as the degree of accuracy is increased.) However, Mullikin<sup>12</sup> has given simple formulas that may be used to calculate upper and lower bounds for  $t_{\rm C}$  for isotropic scattering and any value of m. A computer program was written to calculate these bounds for different m, and the results are presented in columns 4 and 5 of Table I. The final two columns of Table I present critical lengths that Case<sup>6</sup> and Mitsis<sup>8</sup> have obtained for isotropic scattering using different approximate methods. The blanks in these two columns indicate that numerical results were not reported for some values of m.

TABLE I. Dependence of the Critical Length on m (except for column 2, all results are for isotropic scattering)

	t	C	Mulli Boun			
m	Rayleigh	Isotropic	Lower	Upper	Case <sup>6</sup>	Mitsis <sup>8</sup>
1.05	6.589	6.605	6.553	6.684		
1.10	4.214	4.233	4.191	4.286	4.227	4.24
1.30	1.866	1.887	1.857	1.905	1.875	1.780
1.50	1.201	1.221	1.199	1.227	1.209	
1.60	1.014	1.034	1.014	1.039	1.023	1.022
1.80	0.764	0.784	0.771	0.792	0.785	1.022
2.00	0.605	0.623	0.617	0.639	0.640	0.621
2.20	0.493	0.511	0.511	0.534		0.021
2.40	0.411	0.429	0.434	0.459		
2.60	0.348	0.365	0.376	0.403		

Our computations of  $t_c$  for isotropic scattering fall within Mullikin's bounds for  $m \le 2.2$ . However, for m > 2.2, our  $t_c$  is slightly below the lower bound of Mullikin. This indicates that our model should be reasonably accurate for moderate values of m, but for larger m, corresponding to smaller critical lengths, the accuracy of the approximation decreases. Comparing the critical lengths computed by Case and Mitsis, we see that Case's method gives a critical length outside Mullikin's bounds for m = 2.0. However, for smaller m, the lengths are within Mullikin's bounds. Mitsis' result for m = 1.3 is outside the bounds, but the other lengths he reported are within the bounds. Since neither Case nor Mitsis presented values for m > 2.0, comparison between the approximations in this range is difficult. Case's method can, in principle, be calculated to any desired accuracy; however, the zeroth and first-order approximation for which numerical results have been given depend for their accuracy upon m - 1 being small. This assumption, added to the fact that Case's critical

length for m=2.0 is outside Mullikin's bounds, while our method gives results within the bounds for m up to 2.2, suggests that our method is more accurate than Case's for m>2.0. Mitsis' approximation is a modification of Case's and appears to be more accurate than Case's for large m. The values of  $t_{\rm C}$  for Rayleigh scattering are close to, but always slightly less than, the values for isotropic scattering with the same m. The difference between the two lengths stays close to 0.018 as m varies.

### B. The Mean Number of Emergent Particles

From the numerical solution of Eqs. 19 and 20, we obtain the mean number of particles  $M_j(x,i)$  emergent in any direction  $\mu_j$ , conditional on a single initial particle with position x and direction  $\mu_i$ . In the continuous model, the mean number of particles emerging with direction cosines in  $(\mu, \mu + d\mu)$  can be written as  $f(\mu) d\mu$ , where  $f(\mu)$  is the mean density in direction  $\mu$ . The function  $f(\mu)$  can be estimated from the means  $M_j(x,i)$  in the manner described in Ref. 3, p. 99.

Thus, for example, if we consider a single particle incident normally on the right face of the slab (i.e., if we take  $x = t, \mu_i = -1$ ), then the mean density  $f(\mu)$ ,  $0 \le \mu \le 1$ , of the reflected particles is estimated by

$$f(1) = 3.75M_1(t, -1),$$
  
 $f(\mu_i) = 15M_i(t, -1), i = 2, 3, 4,$ 

and

$$f(0) = 0.$$

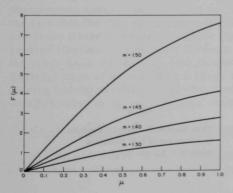


Fig. 2. The Mean Density of Particles Reflected from a Slab of Thickness 1.1 Mean Free Paths When a Single Particle Is Incident Normally on One Face

This function is illustrated in Fig. 2, where it is plotted for t=1.1 and m=1.3, 1.4, 1.45, and 1.50; scattering is assumed to be isotropic. As m approaches the value for which the slab becomes critical ( $m\approx1.55$ ), the mean density begins to increase rapidly.

It is of interest to know how the total number,  $m_{tot}$ , of emergent particles varies with t for fixed m and, in particular, the rate at which  $m_{tot}$  approaches  $\infty$  as t † t<sub>c</sub>. This relationship is shown (again for a single initial particle normally incident on one slab face) for the values m = 1.1, 1.5, 2.0, and 2.473 in Figs. 3, 4, and 5. The results are for

isotropic scattering; those for Rayleigh scattering are similar. Table II compares the results for Rayleigh and isotropic scattering m = 1.05. It

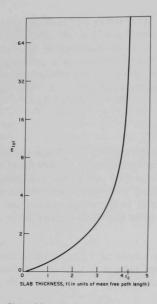


Fig. 3. Mean Number of Emergent Particles as a Function of Slab Thickness When m = 1.1

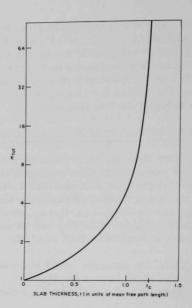
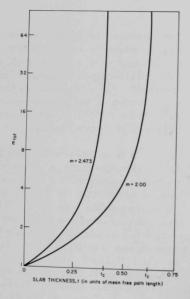


Fig. 4. Mean Number of Emergent Particles as a Function of Slab Thickness When m=1.5



Mean Number of Emergent Particles as a Function of Slab Thickness When m = 2.0 and 2.473

Fig. 5

TABLE II. The Mean Number m<sub>tot</sub> of Emergent Particles When the Mean Number m of Particles per Collision Is 1.05 and the Initial Particle Is Normally Incident on the Slab

Slab Thickness,	Rayleigh Scattering	Isotropic Scattering	Slab Thickness, t	Rayleigh Scattering	Isotropic Scattering
0.1	1.006	1.006	4.3	1.940	1.943
0.3	1.020	1.020	4.5	2.068	2.069
0.5	1.036	1.037	4.7	2.221	2.221
0.7	1.054	1.056	4.9	2.409	2.407
0.9	1.075	1.077	5.1	2.645	2.639
1.1	1.097	1.101	5.3	2.952	2.941
1.3	1.122	1.126	5.5	3.369	3.350
1.5	1.149	1.153	5.7	3.970	3.935
1.7	1.178	1.182	5.9	4.916	4.849
1.9	1.210	1.214	6.1	6.630	6.482
2.1	1.244	1.248	6.3	10.702	10.249
2.3	1.280	1.285	6.5	32.992	28.389
2.5	1.320	1.325	6.55	74.04	
2.7	1.364	1.369	6.587	1,640	
2.9	1.411	1.416	6.589	15,013	
3.1	1.463	1.468	6,589+	00	
3.3	1.520	1.525	6.6		626.5
3.5	1.585	1.589	6.603		1,936
3.7	1.656	1.661	6.604		9,002
3.9	1.738	1.742	6.604+		00
4.1	1.831	1.835	Secretary of the second		

shows that for small values of t,  $m_{tot}$  is larger for isotropic scattering, but for larger values of t,  $m_{tot}$  is larger for Rayleigh scattering. This phenomenon appears to occur for all values of m and is probably due to the fact that for thin slabs the particles resulting from the first collision are more likely to escape from the slab in the Rayleigh case, owing to the greater likelihood of directly forward or directly backward scattering. On the other hand, as the slab gets thicker, there is more chance in the Rayleigh case of establishing a large self-sustaining population of particles moving nearly parallel to the slab faces. This would also explain the smaller value of  $t_{\rm C}$  for Rayleigh scattering.

### C. Calculations of the Second Moments

We now consider the second-moment structure of the first-passage distribution. Three parameters are under consideration:

$$m \left(= \sum_{n=0}^{\infty} n \pi_n \right),$$

the mean number of particles produced per collision;

$$\sigma^2 \left( = \sum_{n=0}^{\infty} (n = m)^2 \pi_n \right),$$

the variance of the number of particles produced per collision; and t, the length of the slab. The second-moment structure varies considerably with the values of these parameters. However, the behavior is essentially the same for Rayleigh as for isotropic scattering.

Equations 30-32 show that the second factorial moments are of the form

$$S_{\alpha\beta}(x,i) = m_{(2)}w_{\alpha\beta}(x,i),$$

where, for given  $m, w_{\alpha\beta}(x, i)$  is independent of  $\sigma^2 = m_{(2)} + m - m^2$ . The covariance of the numbers of particles emergent in directions  $\alpha$  and  $\beta$  is given by

$$\begin{aligned} &\operatorname{Cov}_{\alpha}{}_{\beta}(\mathbf{x},\mathbf{i}) \ = \ & \operatorname{S}_{\alpha}{}_{\beta}(\mathbf{x},\mathbf{i}) \ - \ & \operatorname{M}_{\alpha}(\mathbf{x},\mathbf{i}) \operatorname{M}_{\beta}(\mathbf{x},\mathbf{i}), \qquad \beta \ \neq \ \alpha; \\ &\operatorname{Cov}_{\alpha}{}_{\beta}(\mathbf{x},\mathbf{i}) \ = \ & \operatorname{S}_{\alpha}{}_{\alpha}(\mathbf{x},\mathbf{i}) \ + \ & \operatorname{M}_{\alpha}(\mathbf{x},\mathbf{i}) \ - \ & \operatorname{M}_{\alpha}(\mathbf{x},\mathbf{i})^2, \qquad \beta \ = \ \alpha. \end{aligned}$$

Hence, for fixed m, t, x, and i, the covariance matrix of the numbers of particles emergent in the eight possible directions of motion is a linear function of  $\sigma^2$ . (If m is not an integer,  $\sigma^2$  has a positive minimum possible value, which can easily be calculated.) In particular, the variance  $\sigma^2$  of the total number of emergent particles is a linear function of  $\sigma^2$ ; i.e.,

$$\sigma_{\text{tot}}^2 = \xi + \eta \sigma^2,$$

where  $\xi$  and  $\eta$  depend only on m, t, x, and i.

To illustrate the numerical results, we shall again restrict ourselves to isotropic scattering with a single initial particle incident normally on one face of the slab. More precisely, we shall take  $\mathbf{x}=0$  and  $\mathbf{i}=1$  (recalling from Eq. 6 that  $\mu_1=1$ ).

If  $\pi_n=0$  for  $n\geq 2$ , the second-moment structure of the emergent population is completely determined by the first-moment structure. In fact, the covariance of the numbers emerging in directions  $\alpha$  and  $\beta$  is expressed in terms of the means as follows:

$$\operatorname{Cov}_{\alpha\beta} = -\operatorname{M}_{\alpha}\operatorname{M}_{\beta}$$
 if  $\beta \neq \alpha$ ;  
 $\operatorname{Cov}_{\alpha\beta} = \operatorname{M}\alpha - \operatorname{M}_{\alpha}^2$  if  $\beta = \alpha$ .

We shall therefore not discuss this case any further and assume from now on that

$$\sum_{n=2}^{\infty} \pi_n > 0.$$

A typical example of the behavior when m<1 is given by the case  $\pi_0=0.95$ ,  $\pi_{10}=0.05$ , for which m=0.50,  $\sigma=2.1794$ . The mean and the standard deviation of the number of transmitted particles both converge to 0 as  $t\to\infty$ ; however, the mean and the standard deviation of the number of particles reflected approach nonzero limits as  $t\to\infty$ . Figure 6 shows the

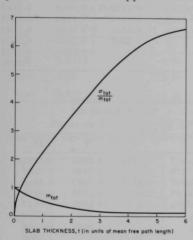


Fig. 6. The Mean and the Coefficient of Variation of the Number of Emergent Particles When m=0.5,  $\sigma=2.1794$ 

dependence of mtot and otot/mtot on the slab thickness, t. Note that although mtot is a decreasing function of t, otot/ mtot increases to its asymptotic value. For t = 0.25, the correlations between emergent direction 1 and the other seven possible emergent directions are small in absolute value (≤0.10) and negative; all the other correlations are positive and in the range 0.35 to 0.60. This is due to the fact that if a particle emerges in direction I there is some indication that no collision has occurred and hence that no other particles emerge from the slab. However, if a particle emerges traveling in a direction other than 1, then a collision must have occurred and there are probably particles emerging in different directions. For t = 0.50, the same qualitative relation exists between the correlations, although all correlations are smaller in absolute value. For larger

values of t, such as t=2.5, all correlations are positive, although the correlations involving direction 1 are still smaller than the others; the largest element is 0.58. For the asymptotic case  $t=\infty$  (which, as far as the reflected particles are concerned, seems to be essentially reached when t=4), the correlations between directions 7, 8, 9, and 10 are all between 0.35 and 0.60.

We now turn to the case m>1. The following describes the general behavior of the correlations for given m and  $\sigma$  as t increases from zero to  $t_C$ . For small t, the correlations are all positive, except for those involving direction 1, which are negative (for the reason explained in the preceding paragraph when m<1). As t increases, the correlations all

increase until, for some value between 0 and  $t_{\rm C}$ , they are all positive. As t gets extremely close to  $t_{\rm C}$ , all the correlations approach 1. To illustrate these effects, Tables III, IV, and V present the correlation matrices for isotropic scattering with m = 1.5 and  $\sigma$  = 0.50; the values of t are 0.5, 0.9, and 1.2 (the critical length  $t_{\rm C}$  is 1.221).

TABLE III. Upper Half of the Correlation Matrix of the Numbers of Particles Emerging in Directions 1, 2, 3, 4, 7, 8, 9, and 10 for Slab Thickness t=0.5

1	2	3	4	7	8	9	10
1 1.000	0 -0.3524	-0.3296	-0.2969	-0.3133	-0.3412	-0.3602	-0.2100
2	1.0000	0.2942	0.2697	0.2542	0.2835	0.3037	0.1778
3		1.0000	0.2575	0.2360	0.2646	0.2844	0.1667
4			1.0000	0.2100	0.2373	0.2563	0.1505
7				1.0000	0.2524	0.2651	0.1543
8					1.0000	0.2906	0.1694
9						1.0000	0.1797
10							1.0000

TABLE IV. Upper Half of the Correlation Matrix of the Numbers of Particles Emerging in Directions 1, 2, 3, 4, 7, 8, 9, and 10 for Slab Thickness t = 0.9

	1	2	3	4	7	8	9	10
1 2 3 4 7 8 9	1.0000	0.3082 1.0000	0.3001 0.7532 1.0000	0.2849 0.7105 0.6903 1.0000	0.2575 0.6870 0.6597 0.6155 1.0000	0.2815 0.7383 0.7102 0.6642 0.6771 1.0000	0.2963 0.7690 0.7407 0.6939 0.6990 0.7458 1.0000	0.2352 0.6087 0.5866 0.5498 0.5517 0.5891 0.6108

TABLE V. Upper Half of the Correlation Matrix of the Numbers of Particles Emerging in Directions 1, 2, 3, 4, 7, 8, 9, and 10 for Slab Thickness t=1.2

	1	2	3	4	7	8	9	10
1 2 3 4 7 8 9	1.0000	0.9977 1.0000	0.9975 0.9989 1.0000	0.9972 0.9985 0.9983 1.0000	0.9970 0.9983 0.9981 0.9977 1.0000	0.9975 0.9988 0.9985 0.9981 0.9983 1.0000	0.9977 0.9990 0.9988 0.9984 0.9985 0.9989 1.0000	0.9965 0.9978 0.9976 0.9972 0.9973 0.9977

The close resemblance between Eqs. 19 and 20 for  $M_{\alpha}(x,i)$  and Eqs. 22 and 23 for  $S_{\alpha\beta}(x,i)$  suggests that the second moments become infinite for the same length  $t_c$  as the first moments. It is of interest to examine how  $\sigma_{tot}$  changes as m,  $\sigma$ , and t vary. As discussed above,  $\sigma_{tot}^2 = \xi + \eta \sigma^2$ , where (for fixed x and i, in particular, for the values x = 0, i = 1, under consideration)  $\xi$  and  $\eta$  depend only on m and t. The quantity  $\xi$  may be thought of as the variance due to the variability in the particle paths, and  $\eta \sigma^2$  as the variance due to the variability in the number of particles produced per collision. Table VI gives the quantities  $\xi$  and  $\eta$  for several values of m and t. (We note again that for nonintegral m, there is a smallest possible positive value of  $\sigma$ , which can easily be calculated.)

TABLE VI.	Values of $\xi$ and	$\eta$ in the Relation $\sigma_{tot}^2$	$= \xi + \eta \sigma^2$ for
a Single	Particle Incident	Normally on a Slab of	Length t

m = 1.10			m = 1.50			m = 2.00			
t	ξ	η	t	ξ	η	t	Ę	η	
1.00	0.0712	2.752	0.50	1.612	3.434	0.25	3.348	2.166	
3.00	7.32	102.8	0.90	39.74	65.01	0.50	212	115.5	
4.15	40,010	372,180	1.20	203,700	275,230	0.60	39,456	20,050	

Figures 7-9 show the relationship between  $\sigma_{tot}/m_{tot}$  and t for isotropic scattering and several values of m and  $\sigma$ . The case m = 2.4730,

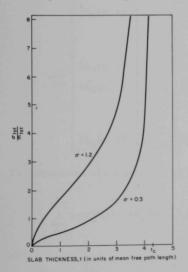


Fig. 7. The Coefficient of Variation of the Number of Emergent Particles When m = 1.1

σ = 1.1051, corresponds to a probability distribution {\pi\_n} reported for neutron fission in U235.15 The graphs all show an inflection point for small values of t. The results indicate that otot/mtot → o as t tc; moreover, otot/mtot reaches the value I for t much smaller than tc. Thus, even for a slab whose length is small compared with tc, the variability in the number of emergent particles is quite large. This conclusion is related to the fact that, even with no multiplication of particles (i.e.,  $\pi_n = 0$  for  $n \ge 2$ ), the variance of the number of collisions experienced by emergent particles is large (c.f. Abu-Shumays1 and Brockwell3).

The graphs corresponding to those in Figs. 7-9 for Rayleigh scattering are similar to the curves for isotropic scattering and are not shown. Of course,  $\sigma_{tot}/m_{tot} \rightarrow \infty \text{ in this case as t $\uparrow$ t_c for Rayleigh scattering, not the value of $t_c$ for isotropic scattering. The similarity of the$ 

two sets of curves indicates that the behavior of  $\sigma_{tot}/m_{tot}$  is insensitive to small changes in the scattering law.

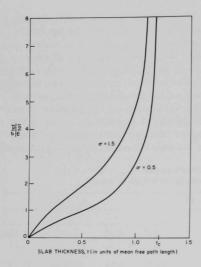


Fig. 8. The Coefficient of Variation of the Number of Emergent Particles When m = 1.5

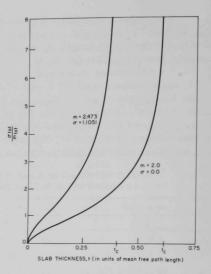


Fig. 9. The Coefficient of Variation of the Number of Emergent Particles When m = 2.0 and 2.473

#### APPENDIX A

### Mathematical Methods Used in the Computer Program

This appendix presents in detail the mathematical methods used in the computer program to calculate the formulas for the means and the second factorial moments; these formulas were given in Eqs. 26 and 32.

First we discuss the computation of  $M_{\alpha}(x,i)$ , the mean number of particles emergent in direction  $\alpha$  ( $\alpha=1,\ldots,4,7,\ldots,10$ ) conditional on a particle at position x ( $0 \le x \le t$ ) traveling in direction i ( $i=1,\ldots,10$ ). We return to the basic Eq. 24; i.e.,

$$\begin{bmatrix} \mu_1 \frac{\partial}{\partial \mathbf{x}} & 0 \\ \vdots \\ 0 & \mu_{10} \frac{\partial}{\partial \mathbf{x}} \end{bmatrix} \begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix} = \begin{bmatrix} \mathbf{1} - \mathbf{m} \mathbf{P}_{1,1} & - \mathbf{m} \mathbf{P}_{1,2} & \dots & - \mathbf{m} \mathbf{P}_{1,10} \\ \vdots \\ -\mathbf{m} \mathbf{P}_{10,1} & \dots & \mathbf{1} - \mathbf{m} \mathbf{P}_{10,10} \end{bmatrix} \begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix}.$$

Since  $\mu_5 = \mu_6 = 0$ , we can rewrite this as Eq. 25,

$$\frac{\partial}{\partial \mathbf{x}} \begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 4) \\ \mathbf{M}_{\alpha}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix} = \mathbf{R} \begin{bmatrix} \mathbf{M}_{\alpha}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 4) \\ \mathbf{M}_{\alpha}(\mathbf{x}, 4) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 7) \\ \vdots \\ \mathbf{M}_{\alpha}(\mathbf{x}, 10) \end{bmatrix}.$$

To determine the elements of the 8 x 8 matrix R, we use the equations

$$\sum_{j=1}^{10} (-mP_{5j}) \cdot M_{\alpha}(x,j) + M_{\alpha}(x,5) = 0$$
 (A.1)

and

$$\sum_{j=1}^{10} (-mP_{6j}) \cdot M_{\alpha}(x,j) + M_{\alpha}(x,6) = 0 \quad (\alpha = 1, ..., 4, 7, ..., 10). \tag{A.2}$$

Therefore,

$$M_{\alpha}(x,5) = \sum_{\substack{j=1\\j\neq 5,6}}^{10} M_{\alpha}(x,j) \left\{ \frac{mP_{5j}(1-mP_{66}) + mP_{56}mP_{6j}}{(1-mP_{55})(1-mP_{66}) - mP_{56}mP_{65}} \right\}$$
(A.3)

and

$$\begin{split} M_{\alpha}(x,6) &= \sum_{\substack{j=1\\j\neq 5,6}}^{10} M_{\alpha}(x,j) \left\{ \frac{mP_{6j}(1-mP_{55}) + mP_{65}mP_{5j}}{(1-mP_{56})(1-mP_{66}) - mP_{56}mP_{65}} \right\} \\ &(\alpha=1,\ldots,4,7,\ldots,10). \end{split} \tag{A.4}$$

So rij, the (i, j)th element of R, is given by

$$\mathbf{r_{ij}} = \frac{-\mathrm{mP_{ij}} - \mathrm{mP_{i5}} \cdot \gamma_5(j) - \mathrm{mP_{i6}} \cdot \gamma_6(j)}{\mu_i}$$

 $(i=1,...,4, j=1,...,4, i \neq j;$  for i=5,...,8 and j=5,...,8, i and j are replaced on the right-hand side of this equation by i+2 and j+2.)

(A-5)

$$\mathbf{r_{ii}} = \frac{1 - \mathbf{mP_{ii}} - \mathbf{mP_{i5}} \cdot \gamma_5(i) - \mathbf{mP_{i6}} \cdot \gamma_6(i)}{\mu_i}$$

(i=1,...,4; for i=5,...,8, i is replaced by i+2 on the right-hand side),

where

$$\gamma_{5}(j) = \frac{mP_{5j}(1 - mP_{66}) + mP_{56}mP_{6j}}{(1 - mP_{55})(1 - mP_{66}) - mP_{56}mP_{65}}$$
(A.6)

and

$$\gamma_6(j) = \frac{mP_{6j}(1 - mP_{55}) + mP_{65}mP_{5j}}{(1 - mP_{55})(1 - mP_{66}) - mP_{56}mP_{65}} \qquad (j = 1, ..., 4, 7, ..., 10).$$
(A.7)

To calculate exp(Rt) as required in Eq. 26, we use the Jordan decomposition of the matrix R. If m, the mean number of particles produced per collision, is not equal to 1, then the eight eigenvalues of R will in general be distinct; in fact, from a certain symmetry of R, one can show that these eigenvalues form four pairs of numbers with opposite signs. However, if m=1, zero is a double eigenvalue of R; this double eigenvalue causes the Jordan decomposition of R to be nondiagonal. Since this non-diagonality complicates the computations, we exclude the case m=1. If, in fact, numerical results are desired for m=1, we can perform the calculations for m=1.0001 and m=0.9999 and average the results, provided the slab is not nearly critical when m=1.0001. (For m=1.0001 and m=0.9999, there will be two eigenvalues close to zero; experience with the numerical routine JACOBI, used to calculate eigenvalues and eigenvectors, has indicated that it can separate these two nonzero eigenvalues for these m, so that the diagonal Jordan decomposition can be achieved numerically.)

Thus, letting T =  $[\underline{t}_1 \dots \underline{t}_8]$  be the matrix of eigenvectors of R, we have

$$\mathbf{T}^{-1}\mathbf{R} \ \mathbf{T} = \begin{bmatrix} \lambda_1 & 0 \\ & \cdot \\ 0 & \lambda_8 \end{bmatrix}, \tag{A.8}$$

where  $\lambda_1,\ldots,\lambda_8$  are the eight distinct eigenvalues of R. The matrices T,  $T^{-1}$ , and the numbers  $\lambda_1,\ldots,\lambda_8$  may be complex. (It seems that if m<1, all eight eigenvalues, and thus the eigenvectors, are real; however, if m>1, there is always one pair of purely imaginary eigenvalues. There are then six real eigenvectors and two other eigenvectors, complex conjugates of each other, with imaginary parts.)

Since

$$\exp(Rt) = I + \sum_{j=1}^{\infty} (Rt)^{j}/j!,$$

it follows that

$$T^{-1} \exp(Rt)T = I + T^{-1}RtT + T^{-1}(Rt)^2T/2! + \dots$$

In terms of the matrix

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 \\ & \cdot \\ & \cdot \\ 0 & \lambda_8 \end{bmatrix},$$

we can write

$$T^{-1} \exp(Rt)T = I + \Lambda t + (\Lambda t)(\Lambda t)/2! + \dots = \exp(\Lambda t);$$

therefore,

$$\exp(Rt) = T \exp(\Lambda t)T^{-1}.$$
 (A.9)

Letting

$$\mathbf{T}^{-1} = \begin{bmatrix} \mathbf{r}_1 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{r}_8 \end{bmatrix},$$

we have

$$\exp(\mathbf{R}\mathbf{x}) = e^{\lambda_1 \mathbf{x}} U_1 + \dots + e^{\lambda_8 \mathbf{x}} U_8, \tag{A.10}$$

where

$$U_i = \underline{t}_i \cdot \underline{r}_i \quad (i = 1, ..., 8).$$
 (A.11)

Each  $U_i$  is an 8 x 8 matrix, since  $\underline{t}_i$  is a column vector and  $\underline{r}_i$  is a row vector. The eight matrices  $U_i$  are computed.

Now let M(x) be the 8 x 8 matrix

$$\begin{bmatrix} M_1(x,1) & \dots & M_4(x,1) & M_7(x,1) & \dots & M_{10}(x,1) \\ \vdots & & & & \vdots \\ M_1(x,4) & & & & & \vdots \\ M_1(x,7) & & & & & & \vdots \\ \vdots & & & & & & & & \\ M_1(x,10) & \dots & & & & & & \\ M_{10}(x,10) & \dots & & & & & \end{bmatrix}$$

Then  $M(t) = \exp(Rt) \cdot M(0)$ , where M(0) is the 8 x 8 matrix determined by the boundary conditions. This matrix was partitioned as

$$\begin{bmatrix} C_1 & C_2 \\ 0 & I \end{bmatrix},$$

and the solutions for  $C_1$  and  $C_2$  were given after Eq. 29. Thus  $\texttt{M}(x) = e^{\lambda_1 x} Z_1 + \ldots + e^{\lambda_8 x} Z_8$  (0  $\leq x \leq$  t), where  $Z_i = U_i \cdot \texttt{M}(0)$  (i = 1, ..., 8). The eight matrices  $Z_i$  are calculated. Now we use the fact that  $M_{\alpha}(x,5)$  and  $M_{\alpha}(x,6)$  are linear combinations of the  $M_{\alpha}(x,j)$  (j = 1, ..., 4, 7, ..., 10;  $\alpha$  = 1, ..., 4, 7, ..., 10) as given in Eqs. A.3 and A.4. Thus, if we let M(x) be the 10 x 8 matrix

$$\begin{bmatrix} M_{1}(x,1) & \dots & M_{4}(x,1) & M_{7}(\lambda,1) & \dots & M_{10}(x,1) \\ \vdots & & & & \vdots \\ M_{1}(x,10) & \dots & M_{4}(x,10) & M_{7}(x,10) & \dots & M_{10}(x,10) \end{bmatrix}. \tag{A.12}$$

then M(x) =  $e^{\lambda_1 x}$   $W_1$  + ... +  $e^{\lambda_8 x}$   $W_8$ , where the  $W_1$  are all 10 x 8 matrices, and

$$\begin{aligned} & W_{\mathbf{q}}(\mathbf{i},\mathbf{j}) = Z_{\mathbf{q}}(\mathbf{i},\mathbf{j}) & \quad (\mathbf{i} = 1, \dots, 4; \ \mathbf{j} = 1, \dots, 8), \\ & W_{\mathbf{q}}(\mathbf{i} + 2,\mathbf{j}) = Z_{\mathbf{q}}(\mathbf{i},\mathbf{j}) & \quad (\mathbf{i} = 5, \dots, 8; \ \mathbf{j} = 1, \dots, 8), \\ & W_{\mathbf{q}}(5,\mathbf{j}) = \sum_{k=1}^{4} \gamma_{5}(\mathbf{k}) Z_{\mathbf{q}}(\mathbf{k},\mathbf{j}) + \sum_{k=5}^{8} \gamma_{5}(\mathbf{k} + 2) \ Z_{\mathbf{q}}(\mathbf{k},\mathbf{j}) & \quad (\mathbf{j} = 1, \dots, 8), \\ & W_{\mathbf{q}}(6,\mathbf{j}) = \sum_{k=1}^{4} \gamma_{6}(\mathbf{k}) Z_{\mathbf{q}}(\mathbf{k},\mathbf{j}) + \sum_{k=5}^{8} \gamma_{6}(\mathbf{k} + 2) \ Z_{\mathbf{q}}(\mathbf{k},\mathbf{j}) & \quad (\mathbf{j} = 1, \dots, 8) \\ & \qquad (\mathbf{q} = 1, \dots, 8), \end{aligned}$$

and  $\gamma_5(k),\,\gamma_6(k)$  are defined by Eqs. A.6 and A.7. The eight matrices W are computed. These matrices completely determine the 10 x 8 matrix M(x), which gives the mean number of particles emergent in each of the eight possible emergent directions for a particle at position x traveling in each of the 10 possible directions of motion. The eight W's, eight U's and eight  $\lambda$ 's are all stored for use in the second part of the program.

Now we consider Eq. 30, the basic equation for the second factorial moments:

$$\begin{bmatrix} \mu_{1} \frac{\partial}{\partial \mathbf{x}} & 0 \\ & \ddots & \\ & & \ddots & \\ & & & \\ 0 & \mu_{10} \frac{\partial}{\partial \mathbf{x}} \end{bmatrix} \begin{bmatrix} \mathbf{S}_{\alpha \beta}(\mathbf{x}, 1) \\ & \ddots & \\ & & & \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 10) \end{bmatrix} = \begin{bmatrix} \mathbf{1} - \mathbf{m} \mathbf{P}_{1,1} - \mathbf{m} \mathbf{P}_{1,2} \dots - \mathbf{m} \mathbf{P}_{1,10} \\ & \ddots & & \\ & & & \\ - \mathbf{m} \mathbf{P}_{10,1} \dots & & \mathbf{1} - \mathbf{m} \mathbf{P}_{10,10} \end{bmatrix} \begin{bmatrix} \mathbf{S}_{\alpha \beta}(\mathbf{x}, 1) \\ & \ddots & \\ & & \\ \mathbf{S}_{\alpha \beta}(\mathbf{x}, 10) \end{bmatrix}$$

$$-\mathbf{m}_{(z)}\begin{bmatrix} \mathbf{F}_{\alpha\beta}(\mathbf{x},1) \\ \vdots \\ \mathbf{F}_{\alpha\beta}(\mathbf{x},10) \end{bmatrix}.$$

We recall that

$$\mathbf{F}_{\alpha\,\beta}(\mathbf{x},\ell) \; = \left\{ \sum_{\mathbf{k}=1}^{40} \; \mathbf{M}_{\alpha}(\mathbf{x},\mathbf{k}) \mathbf{P}_{\ell\mathbf{k}} \right\} \cdot \left\{ \sum_{\mathbf{k}=1}^{10} \; \mathbf{M}_{\beta}(\mathbf{x},\mathbf{k}) \mathbf{P}_{\ell\mathbf{k}} \right\}$$

$$(\alpha = 1, ..., 4, 7, ..., 10; \beta = 1, ..., 4, 7, ..., 10; \ell = 1, ..., 10).$$

The first factor can be thought of as the  $\ell$ th row of the matrix P multiplied by the column vector  $\underline{M}_{\alpha}(\mathbf{x})$ ; writing  $\underline{M}_{\alpha}(\mathbf{x},\ell)$  in terms of the W's, we get

$$F_{\alpha\,\beta}(x,\ell) = \left\{ \sum_{k=1}^{10} \, P_{\ell \, k} \, \, \sum_{q=1}^{8} \, \mathrm{e}^{\lambda q \, x} \, W_q(k,\,\alpha) \right\} \, \cdot \, \left\{ \, \sum_{m=1}^{10} \, P_{\ell \, m} \, \, \, \sum_{r=1}^{8} \, \mathrm{e}^{\lambda r \, x} W_r(m,\,\beta) \right\}$$

 $(\alpha=1,\ldots,4,\ \beta=1,\ldots,4,\ \ell=1,\ldots,10;\ \text{for }\alpha\text{ and }\beta=7,\ldots,10,$   $\alpha$  and  $\beta$  are replaced by  $\alpha-2$  and  $\beta-2$  on the right-hand side).

This equation can be written

$$F_{\alpha\beta}(\mathbf{x},\ell) = \sum_{q=1}^{8} \sum_{\mathbf{r}=1}^{8} e^{(\lambda_{q} + \lambda_{\mathbf{r}})\mathbf{x}} \cdot X_{\alpha\beta_{q}\mathbf{r}}(\ell), \tag{A.14}$$

where

$$\begin{split} \mathbf{X}_{\alpha\beta\mathbf{qr}}(\ell) &= \sum_{\mathbf{k}=1}^{10} \mathbf{P}_{\ell\mathbf{k}} \mathbf{W}_{\mathbf{q}}(\mathbf{k},\alpha) \cdot \sum_{\mathbf{m}=1}^{10} \mathbf{P}_{\ell\mathbf{m}} \mathbf{W}_{\mathbf{r}}(\mathbf{m},\beta) \\ &(\alpha=1,\ldots,4,\ \beta=1,\ldots,4,\ \ell=1,\ldots,10;\ \text{for }\alpha \text{ and }\beta=7,\ldots,10,\\ &\alpha-2 \text{ and }\beta-2 \text{ replace }\alpha \text{ and }\beta \text{ on the right side}). \end{split}$$

The X's are calculated.

Next we change the form of the basic equation to that of Eq. 31, i.e.,

$$\frac{\partial}{\partial \mathbf{x}} \begin{bmatrix} \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 4) \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 7) \\ \vdots \\ \vdots \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 10) \end{bmatrix} = \mathbf{R} \begin{bmatrix} \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 4) \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 4) \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 7) \\ \vdots \\ \vdots \\ \mathbf{S}_{\alpha \, \beta}(\mathbf{x}, 10) \end{bmatrix} + \begin{bmatrix} \mathbf{V}_{\alpha \, \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{V}_{\alpha \, \beta}(\mathbf{x}, 1) \\ \vdots \\ \mathbf{V}_{\alpha \, \beta}(\mathbf{x}, 8) \end{bmatrix} .$$

by using the fact that  $\mu_5$  =  $\mu_6$  = 0. The 8 x 8 matrix R is the same as in Eq. A.5, and elementary algebra shows that

$$V_{\alpha\beta}(\mathbf{x},\ell) = \left[ F_{\alpha\beta}(\mathbf{x},\ell) + \frac{\mathrm{mP}_{\ell 5}(1-\mathrm{mP}_{66}) + \mathrm{mP}_{\ell 6}\mathrm{mP}_{65}}{(1-\mathrm{mP}_{55})(1-\mathrm{mP}_{66}) - \mathrm{mP}_{56}\mathrm{mP}_{65}} F_{\alpha\beta}(\mathbf{x},5) \right] \\ + \frac{\mathrm{mP}_{\ell 6}(1-\mathrm{mP}_{55}) + \mathrm{mP}_{\ell 5}\mathrm{mP}_{56}}{(1-\mathrm{mP}_{55})(1-\mathrm{mP}_{66}) - \mathrm{mP}_{56}\mathrm{mP}_{65}} F_{\alpha\beta}(\mathbf{x},6) \right] \frac{-\mathrm{m}(\mathbf{z})}{\mu\ell} \\ (\alpha=1,\ldots,4,\beta=1,\ldots,4,\ell=1,\ldots,4; \text{ similar equations hold for } \\ \alpha=7,\ldots,10,\beta=7,\ldots,10, \text{ and } \ell=5,\ldots,8).$$
(A.16)

This can be simplified to

$$V_{\alpha\beta}(\mathbf{x},\ell) = \sum_{\mathbf{q}=1}^{8} \sum_{\mathbf{r}=1}^{8} e^{(\lambda_{\mathbf{q}} + \lambda_{\mathbf{r}})\mathbf{x}} \cdot Y_{\alpha\beta\mathbf{q}\mathbf{r}}(\ell), \tag{A.17}$$

where

$$Y_{\alpha\beta qr}(\ell) = \left\{ X_{\alpha\beta qr}(\ell) + K_{5}(\ell) \cdot X_{\alpha\beta qr}(5) + K_{6}(\ell) \cdot X_{\alpha\beta qr}(6) \right\} \frac{-m_{(2)}}{\mu\ell}$$

$$(\alpha = 1, ..., 4, ..., 7, ..., 10, \beta = 1, ..., 4, ..., 7, ..., 10, \ell = 1, ..., 4;$$
for  $\ell = 5, ..., 8$ , the  $\ell$  in  $X$  and in  $\mu\ell$  is replaced by  $\ell + 2$ ) (A.18)

and

$$K_{5}(\ell) = \frac{\text{mPl}_{5}(1 - \text{mP}_{66}) + \text{mPl}_{6}\text{mP}_{65}}{(1 - \text{mP}_{55})(1 - \text{mP}_{66}) - \text{mP}_{56}\text{mP}_{65}}$$

$$(\ell = 1, ..., 4; \text{ for } \ell = 5, ..., 8, \ \ell \text{ is replaced by } \ell + 2), \tag{A.19}$$

$$K_{6}(\ell) = \frac{mP_{\ell 6}(1 - mP_{55}) + mP_{\ell 5}mP_{56}}{(1 - mP_{55})(1 - mP_{66}) - mP_{56}P_{65}}$$

$$(\ell = 1, ..., 4; \text{ for } \ell = 5, ..., 8, \ \ell \text{ is replaced by } \ell + 2). \tag{A.20}$$

The K's and the Y's are computed. Now the solution is

$$\begin{bmatrix} S_{\alpha\beta}(\mathbf{x}, 1) \\ \vdots \\ S_{\alpha\beta}(\mathbf{x}, 4) \\ S_{\alpha\beta}(\mathbf{x}, 7) \\ \vdots \\ S_{\alpha\beta}(\mathbf{x}, 10) \end{bmatrix} = \exp(\mathbf{R}\mathbf{x}) \left\{ g_{\alpha\beta} + \int_{0}^{\mathbf{x}} \exp(-y\mathbf{R}) \sum_{q=1}^{8} \sum_{\mathbf{r}=1}^{8} y_{\alpha\beta q} \cdot e^{(\lambda_{q} + \lambda_{\mathbf{r}})y} dy \right\}.$$

$$\vdots$$

$$S_{\alpha\beta}(\mathbf{x}, 10)$$

$$S_{\alpha\beta}(\mathbf{x}, 10)$$

$$\vdots$$

$$S_{\alpha\beta}(\mathbf{x}, 10)$$

Next we write exp(-yR) as

$$\sum_{s=1}^{8} e^{-\lambda_s y} U_s.$$

Then the integral in Eq. A.21 can be written as

$$\sum_{s=1}^{8} \sum_{q=1}^{8} \sum_{r=1}^{8} U_{s} \cdot Y_{\alpha\beta q r} \cdot \int_{0}^{x} e^{(\lambda_{q} + \lambda_{r} - \lambda_{s}) y} dy.$$
 (A.22)

Now the reason for breaking up

$$\int_0^{x} \exp(-yR) \cdot Y_{\alpha\beta}(y) dy$$

into the triple summation of Eq. A.22 is apparent, since

$$\int_0^{x} e^{(\lambda_q + \lambda_r - \lambda_s) y} dy$$

can be integrated analytically. Therefore the solution is

$$\begin{bmatrix} S_{\alpha\beta}(x,1) \\ \vdots \\ S_{\alpha\beta}(x,4) \\ S_{\alpha\beta}(x,7) \\ \vdots \\ S_{\alpha\beta}(x,10) \end{bmatrix} = \exp(xR) \left\{ \underbrace{s_{\alpha\beta} + \sum_{s=1}^{8} \sum_{q=1}^{8} \sum_{r=1}^{8} U_{s} \cdot \underbrace{Y_{\alpha\beta qr} \cdot \left[ \frac{e^{(\lambda_{q} + \lambda_{r} - \lambda_{s})x} - 1}{\lambda_{q} + \lambda_{r} - \lambda_{s}} \right]} \right\}}. (A.23)$$

assuming  $\lambda_q + \lambda_r - \lambda_s \neq 0$  (s=1,...,8; q=1,...,8; r=1,...,8); the eight-component vector  $c_{\alpha\beta}$  is determined by the boundary conditions. Since  $s_{\alpha\beta}(0) = s_{\alpha\beta}(0)$ , the bottom four components of  $s_{\alpha\beta}(0) = s_{\alpha\beta}(0)$ .

The symmetry of directions 1, ..., 4 with directions 10, ..., 7 shows that the  $S_{\alpha\beta}$ 's need only be calculated for  $\alpha=1,\ldots,4$  and  $\beta=1,\ldots,4$ , 7, ..., 10; the symmetry relations are  $S_{\alpha\beta}(\mathbf{x},\ell)=S_{11-\alpha,11-\beta}(\mathbf{t}-\mathbf{x},11-\ell)$  and  $S_{\alpha\beta}(\mathbf{x},\ell)=S_{\beta\alpha}(\mathbf{x},\ell)$  ( $\alpha=1,\ldots,4,7,\ldots,10$ ;  $\beta=1,\ldots,4,7,\ldots,10$ ;  $\ell=1,\ldots,4$ ;  $0\leq\mathbf{x}\leq\mathbf{t}$ ). Thus a complete solution is obtained by evaluating  $S_{\alpha\beta}(\mathbf{x},\ell)$  for  $\alpha=1,\ldots,4$ ,  $\beta=1,\ldots,4$ , 7, ..., 10, and  $\ell=1,\ldots,4$ , 7, ..., 10 ( $0\leq\mathbf{x}\leq\mathbf{t}$ ). Let  $S(\mathbf{x})$  be the 8 x 32 matrix

$$\begin{bmatrix} S_{11}(x,1) \dots S_{14}(x,1) S_{17}(x,1) \dots S_{1,10}(x,1) S_{21}(x,1) \dots S_{2,10}(x,1) S_{31}(x,1) \dots S_{4,10}(x,1) \\ \vdots \\ S_{11}(x,4) \\ S_{11}(x,7) \\ \vdots \\ S_{11}(x,10) \dots \\ \end{bmatrix}, (A.24)$$

and let 
$$\begin{bmatrix} Intl(x)\\ Int2(x) \end{bmatrix}$$
 be the 8 x 32 matrix

$$[\operatorname{Int}_{1,1}(x)\operatorname{Int}_{1,2}(x)\ldots\operatorname{Int}_{1,4}(x)\operatorname{Int}_{1,7}(x)\ldots\operatorname{Int}_{1,10}(x)\operatorname{Int}_{2,1}(x)\ldots\operatorname{Int}_{4,10}(x)],$$

where  $\operatorname{Int}_{\alpha\beta}(x)$  is the eight-component column vector

$$\sum_{s=1}^{8} \sum_{q=1}^{8} \sum_{r=1}^{8} U_{s} \cdot \underline{Y}_{\alpha\beta qr} \cdot \left[ \frac{e^{\left(\lambda_{q} + \lambda_{r} - \lambda_{s}\right)x} - 1}{\lambda_{q} + \lambda_{r} - \lambda_{s}} \right]. \tag{A.25}$$

Thus Intl(x) and Int2(x) are each 4 x 32 matrices. Finally, let C be the 4 x 32 matrix

$$\begin{bmatrix} \mathbb{C}_{11} \cdots \mathbb{C}_{14} \mathbb{C}_{17} \cdots \mathbb{C}_{1,10} \mathbb{C}_{21} \cdots \mathbb{C}_{4,10} \end{bmatrix}$$

where the  $g_{\alpha\beta}$ 's are the top four (i.e., nonzero) components of the  $g_{\alpha\beta}$ 's used in Eq. A.23.

Then we have the equation

$$S(x) = \exp(Rx) \left\{ \begin{bmatrix} C \\ 0 \end{bmatrix} + \begin{bmatrix} Int1(x) \\ Int2(x) \end{bmatrix} \right\}. \tag{A.26}$$

To compute C, we use the boundary conditions on S(t); i.e.,  $S_{\alpha\beta}(t,\ell)=0$   $(\alpha=1,\ldots,4,\ \beta=1,\ldots,4,7,\ldots,10,\ \ell=1,\ldots,4)$ . Thus we compute

$$\begin{bmatrix} Int l(t) \\ Int 2(t) \end{bmatrix}$$

using Eq. A.25. Then letting

$$\exp(Rt = \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix},$$

we have

$$0 = E_{11} \cdot [C + Int1(t)] + E_{12}[Int2(t)]. \tag{A.27}$$

Therefore, C =  $-E_{11}^{-1}E_{12}$  Int2(t) - Int1(t). The 4 x 32 matrix C is computed using this formula. Then S(x) can be calculated for arbitrary x (0  $\leq$  x  $\leq$  t) using Eqs. A.26 and A.25.

The transformations from the second factorial moments  $\mathcal{S}$  to the more meaningful variances, covariances, correlations, and standard deviations are then made using the standard formulas.

It has been observed that the method of calculation becomes numerically unstable when t gets very close to the critical length  $t_{\rm C}$  ( $t_{\rm C}$ -  $t\approx 0.001$ ). A similar phenomenon occurred in the nonmultiplicative case (Brockwell³) when t becomes large (approximately seven mean free paths). However, in the nonmultiplicative case, the range of accuracy was increased considerably by considering thick slabs to be superpositions of thinner slabs (see Ref. 3, Chapter VI, Section 5). An analogous approach could be used to study thick slabs in the multiplicative case, but so far this approach has not been investigated.

## APPENDIX B

## Listing of Computer Program

```
OS/360 FORTRAN H DATE 68.261/22.11.32
LEVEL 15 ( 1 JAN 68)
          COMPILER OPTIONS - NAME= MAIN, OPT=00, LINECNT=57, SOURCE, EBCDIC, NOLIST, NODECK,
                                                                         LOAD, MAP, NOEDIT, ID, NOXREF
                       STOCHASTIC TRANSPORT PROGRAM II
                C
                       IMPLICIT REAL *8(A-H, 0-Z)
ISN 0002
                       REAL*8 LENGTH, M, M2, MU, KAPPA5, KAPPA6
ISN 0003
                      COMPLEX*16 COMP, CR, CT, CTEMP, CTINV, D, DETERM, E11, 1 E12, FACTOR, INT, INT1, INT2, MEAN, SCONST, SMOP, THETA,
ISN 0004
                      2 U, VTEMP, W, XTEMP1, XTEMP2, XX, Y, Z
                      DIMENSION B2(4), COMP(10,10), CONST(8,8), CORR(8,8),

1 CR(8,8), CT(8,8), CTEMP(8,8), CTINV(8,8), D(4,4), E11(4,4),

2 E12(4,4), GAM5(10), GAM6(10), INT(8,32), INT1(4,32),
ISN 0005
                      2 E12(4,4); GAMS(10); KAPPA6(10); MEAN(10,8); MU(10);
3 INT2(4,32); KAPPA5(10); KAPPA6(10); MEAN(10,8); MU(10);
4 OCCOV(8,32); OMEAN(10,8); P(10,10); R(8,8); RR(8,8);
5 RSC(8,32); SCAT(9); SCONST(8,32); SDEV(8); SML(4,32);
6 SMDP(8,32); T(8,8); THETA(8); U(8,8,8); VAR(4,8); VTEMP(8);
                      6 SMOP(8,32),
7 W(8,10,8)
                         W(8,10,8), XX(4,8,8,8,10), Y(4,8,8,8,8), Z(8,8,8)
                      FIVE = 5.0
ISN 0006
                       MU(1) = 1.0
ISN 0007
                       MU(2) = (DSQRT(FIVE) + 1.0)/4.0
ISN 0008
ISN 0009
                       MU(3) = 0.5
                       MU(4) = (DSQRT(FIVE) - 1.0)/4.0
ISN 0010
                       MU(5) = 0.0
ISN 0011
ISN 0012
                      DO 102 I = 1,5
ISN 0013
                  102 \text{ MU(11-I)} = -\text{MU(I)}
                       READ (5,902) ISCAT
ISN 0014
                       IF (ISCAT) 103,106,108
ISN 0015
                       IF ISCAT = 0, ISUTROPIC SCATTERING; IF ISCAT = -1, RAYLEIGH
                C
               C
                       SCATTERING; IF ISCAT = +1, A DIFFERENT SCATTERING LAW IS READ IN.
ISN 0016
                  103 \text{ SCAT}(1) = 0.050
ISN 0017
                      SCAT(2) = (11.0 + DSQRT(FIVE))/320.0
ISN 0018
                       SCAT(3) = 1.0/32.0
                       SCAT(4) = (11.0 - DSQRT(FIVE))/320.0
ISN 0019
ISN 0020
                       SCAT(5) = 0.0250
ISN 0021
                      DO 104 I = 6,9
ISN 0022
                  104 \text{ SCAT(I)} = \text{SCAT(10-I)}
ISN 0023
                      WRITE (6,835)
ISN 0024
                       GO TO 109
ISN 0025
                  106 DO 107 I=1,9
                  107 SCAT(I) = 1.0/30.0
ISN 0026
ISN 0027
                      WRITE (6,837)
ISN 0028
                       GU TO 109
                  108 READ (5,900) (SCAT(I), I=1,9)
ISN 0029
ISN 0030
                  109 CONTINUE
               C
               C
                       COMPUTATION OF MATRIX P
               C
ISN 0031
                       P(1,1) = SCAT(1)
ISN 0032
                       P(1,2) = 4.0*SCAT(2)
ISN 0033
                       P(1,3) = 4.0*SCAT(3)
ISN 0034
                       P(1,4) = 4.0*SCAT(4)
ISN 0035
                       P(2,1) = SCAT(2)
ISN 0036
                      P(2,2) = SCAT(1) + SCAT(2) + SCAT(3) + SCAT(4)
ISN 0037
                      P(2,3) = SCAT(2) + SCAT(3) + SCAT(4) + SCAT(5)
ISN 0038
                      P(2,4) = SCAT(2) + SCAT(3) + SCAT(5) + SCAT(6)
ISN 0039
                      P(3,1) = SCAT(3)
ISN 0040
                      P(3,2) = P(2,3)
ISN C041
                      P(3,3) = SCAT(1) + SCAT(2) + SCAT(6) + SCAT(7)
ISN 0042
                      P(3,4) = SCAT(2) + SCAT(4) + SCAT(5) + SCAT(7)
ISN 0043
                      P(4,1) = SCAT(4)
ISN 0044
                      P(4,2) = P(2,4)
ISN 0045
                     P(4,3) = P(3,4)
```

```
P(4,4) = SCAT(1) + SCAT(3) + SCAT(6) + SCAT(8)
ISN 0046
ISN 0047
                   DO 110 I=7,10
ISN 0048
                   DO 110 J=7,10
ISN 0049
               110 P(I,J) = P(11-I,11-J)
ISN 0050
                   P(7,1) = SCAT(6)
ISN 0051
                   P(7,2) = SCAT(4) + SCAT(5) + SCAT(7) + SCAT(8)
ISN 0052
                   P(7,3) = SCAT(3) + SCAT(5) + SCAT(6) + SCAT(8)
ISN 0053
                   P(7,4) = SCAT(2) + SCAT(4) + SCAT(7) + SCAT(9)
ISN 0054
                   P(8,1) = SCAT(7)
ISN 0055
                   P(8,2) = SCAT(5) + SCAT(6) + SCAT(7) + SCAT(8)
ISN 0056
                   P(8,3) = SCAT(3) + SCAT(8) + SCAT(4) + SCAT(9)
ISN 0057
                   P(8,4) = SCAT(3) + SCAT(5) + SCAT(6) + SCAT(8)
                   P(9,1) = SCAT(8)
ISN 0058
ISN 0059
                    P(9,2) = SCAT(6) + SCAT(7) + SCAT(8) + SCAT(9)
ISN 0060
                    P(9,3) = SCAT(5) + SCAT(6) + SCAT(7) + SCAT(8)
ISN 0061
                   P(9,4) = SCAT(4) + SCAT(5) + SCAT(7) + SCAT(8)
ISN 0062
                    P(10,1) = SCAT(9)
ISN 0063
                    P(10,2) = 4.0*SCAT(8)
ISN 0064
                    P(10,3) = 4.0*SCAT(7)
ISN 0065
                    P(10,4) = 4.0*SCAT(6)
ISN 0066
                   DO 115 I=1,4
ISN 0067
                   DO 115 J=7,10
ISN 0068
               115 P(I,J) = P(11-I,11-J)
ISN 0069
                   P(5,1) = SCAT(5)
ISN 0070
                    P(5,2) = 2.0*SCAT(4) + 2.0*SCAT(6)
ISN 0071
                    P(5,3) = 2.0*SCAT(2) + 2.0*SCAT(8)
                    P(5,4) = 2.0*SCAT(3) + 2.0*SCAT(7)
ISN 0072
ISN 0073
                    P(6,1) = SCAT(5)
                    P(6,2) = 2.0*SCAT(3) + 2.0*SCAT(7)
ISN 0074
ISN 0075
                    P(6,3) = 2.0*SCAT(4) + 2.0*SCAT(6)
ISN 0076
                    P(6,4) = 2.0*SCAT(2) + 2.0*SCAT(8)
                    DO 120 I=5,6
ISN 0077
ISN 0078
                    DO 120 J=7,10
ISN 0079
                120 P(I,J) = P(I,11-J)
ISN 0080
                   P(1,5) = 2.0*SCAT(5)
                    P(1,6) = P(1,5)
ISN 0081
                    P(2,5) = SCAT(4) + SCAT(6)
ISN 0082
                    P(2,6) = SCAT(3) + SCAT(7)
ISN 0083
                    P(3,5) = SCAT(2) + SCAT(8)
ISN 0084
                    P(3,6) = SCAT(4) + SCAT(6)
ISN 0085
                   P(4,5) = SCAT(3) + SCAT(7)
ISN 0086
                    P(4,6) = SCAT(2) + SCAT(8)
ISN 0087
                    P(5,5) = SCAT(1) + SCAT(9)
ISN 0088
ISN 0089
                    P(5,6) = 2.0*SCAT(5)
                    P(6,5) = P(5,6)
ISN 0090
                    P(6,6) = P(5,5)
ISN 0091
                    DO 125 I=7,10
ISN 0092
                    DO 125 J=5,6
ISN 0093
                125 P(I,J) = P(11-I,J)
ISN 0094
                    WRITE (6,905)
ISN 0095
                    WRITE (6,910) ((P(I,J),J=1,10),I=1,10)
ISN 0096
              C
                    READ IN M, M2, AND NUMBER OF LENGTHS FOR THIS MEAN
              C
                130 READ (5,880) M,M2, NUMLTH
ISN 0097
                    IF (M .LE. 0.0) GO TO 500
ISN 0098
                    COMPUTATION OF MATRIX R
              C
                    DEN = (M*P(5,5) - 1.0) *(M*P(6,6) - 1.0) - (M*P(6,5))*(M*P(5,6))
ISN 0100
                    DU 140 I=1,4
ISN 0101
                    GAM6(I) = ((M*P(6,5))*(M*P(5,I)) - (M*P(6,I))*(M*P(5,5)-1.0))/DEN
ISN 0102
                    GAM6(I+6) = ((M*P(6,5))*(M*P(5,I+6)) - (M*P(6,I+6))*(M*P(5,5)-1.0)
ISN 0103
                   1)/DEN
                    GAM5(I) = ((M*P(5,6))*(M*P(6,I)) - (M*P(5,I))*(M*P(6,6)-1.0))/DEN
ISN 0104
                    GAM5(I+6) = (M*P(5,6)*(M*P(6,I+6)) - (M*P(5,I+6))*(M*P(6,6)-1.0))
ISN 0105
                   1/DEN
                140 CONTINUE
ISN 0106
ISN 0107
                    00 150 I=1,4
                    DO 150 J=1.4
ISN 0108
                    R(I,J) = (-M*P(I,J) - M*P(I,5)*GAM5(J) - M*P(I,6)*GAM6(J))/MU(I)
ISN 0109
```

```
R(I,J+4) = (-M*P(I,J+6) - M*P(I,5)*GAM5(J+6) - M*P(I,6)*GAM6(J+6))
ISN 0110
                   R(1+4,J) = (-M*P(1+6,J) - M*P(1+6,5)*GAM5(J) - M*P(1+6,6)*GAM6(J))/
                   1/MU(I)
ISN 0111
                   R(1+4,J+4) = (-M*P(I+6,J+6) - M*P(I+6,5)*GAM5(J+6)-M*P(I+6,6)*GAM6
                   1MU(1+6)
ISN 0112
                   1(J+6))/MU(I+6)
               150 CONTINUE
ISN 0113
                    DO 155 I= 1,4
ISN 0114
                    R(I,I) = R(I,I) + (1.0/MU(I))
                    R(I+4,I+4) = R(I+4,I+4) + (1.0/MU(I+6))
ISN 0115
ISN 0116
                155 CONTINUE
ISN 0117
                    WRITE (6,915)
                    WRITE (6,975) ((R(I,J),J=1,8),I=1,8)
ISN 0118
ISN 0119
                    DO 170 I=1,8
ISN 0120
                    DO 170 J=1,8
ISN 0121
                170 RR(I,J) = R(I,J)
ISN 0122
              C
                     COMPUTATION OF EIGENVALUES & EIGENVECTORS
              C
                    KONST = 1
ISN 0123
                    CALL CLOCK (T1)
ISN 0124
                    CALL JACOBI (RR, T, 8, KONST, 8)
ISN 0125
                    CALL CLOCK(T2)
ISN 0126
                    TT = T2 - T1
ISN 0127
                    WRITE (6,945) KONST,TT
ISN 0128
                    WRITE (6,950)
 ISN 0129
                    WRITE (6,965) ((RR(I,J),J=1,8),I=1,8)
ISN 0130
                    WRITE (6,960)
ISN 0131
                    WRITE (6,965) ((I(I,J),J=1,8),I=1,8)
 ISN 0132
                    IDUM = 0
 ISN 0133
                    DO 180 I=1,7
 ISN 0134
                    IF (IDUM .NE.1) GO TO 171
 ISN 0135
                    IDUM = 0
 ISN 0137
                    GO TO 180
 ISN 0138
                171 IF (DABS(RR(I,I+1)) .GE. 1.00-07) GO TO 174
 ISN 0139
                     THETA (I) = RR(I,I)
 ISN 0141
                    DO 172 J=1,8
 ISN 0142
                172 \text{ CT}(J,I) = T(J,I)
 ISN 0143
                    GO TO 180
 ISN 0144
                174 IF (DABS(RR(I,I)) .LE. 1.0D-07) GO TO 175
 ISN 0145
                     THETA(I) = RR(I,I)
 ISN 0147
                     THETA(I) = THETA(I) + (0.0,1.0)*RR(I,I+1)
 ISN 0148
                     THETA(I+1) = RR(I+1,I+1)
 ISN 0149
                     THETA(I+1) = THETA(I+1) + (0.0,1.0)*RR(I+1,I)
 ISN 0150
                    GO TO 176
 ISN 0151
                175 THETA(I) = RR(I,I+1)*(0.0,1.0)
 ISN 0152
                     THETA(I+1) = RR(I+1,I)*(0.0,1.0)
 ISN 0153
                176 DO 178 J=1,8
 ISN 0154
                     CT(J,I) = T(J,I)
 ISN 0155
                     CT(J,I) = CT(J,I) + (C.O,1.0)*T(J,I+1)
 ISN 0156
                     CT(J,I+1) = T(J,I)
 ISN 0157
                178 \text{ CT}(J,I+1) = \text{CT}(J,I+1) - (0.0,1.0)*T(J,I+1)
 ISN 0158
                     IDUM = 1
 ISN 0159
                180 CONTINUE
 ISN 0160
                     IF (DABS(RR(7,8)) .GE. 1.0D-07) GO TO 183
 ISN 0161
 ISN 0163
                     THETA(8) = RR(8,8)
                     DO 182 J=1,8
 ISN 0164
 ISN 0165
                182 \text{ CT}(J,8) = T(J,8)
                 183 DO 184 I=1,8
 ISN 0166
                     DO 184 J=1,8
 ISN 0167
 ISN 0168
                 184 \text{ CTINV}(I,J) = \text{CT}(I,J)
 ISN 0169
                     WRITE (6,955)
 ISN 0170
                     WRITE (6,908) (THETA(I), I=1,8)
              C
              C
                     CHECK OF DIAGONALIZATION, AND COMPUTATION OF THE 8 U'S
              C
                     CALL MATINV(CTINV, 8, SDEV, 0, DETERM, 8)
 ISN 0171
 ISN 0172
                     WRITE (6,960)
 ISN 0173
                     WRITE (6,964) ((CT(I,J),J=1,8),I=1,8)
                     WRITE (6,970)
 ISN 0174
 ISN 0175
                     WRITE (6,964) ((CTINV(I,J),J=1,8),I=1,8)
```

```
ISN 0176
                    DO 185 I=1,8
ISN 0177
                    DO 185 J=1,8
ISN 0178
                185 CR(I,J) = R(I,J)
ISN 0179
                    CALL CMTMLT (CTINV,8,8,CR,8,8,CTEMP)
ISN 0180
                    CALL CMTMLT (CTEMP, 8, 8, CT, 8, 8, CR)
ISN 0181
                    WRITE (6,920)
ISN 0182
                    WRITE (6,964) ((CR(I,J),J=1,8),I=1,8)
ISN 0183
                    DO 187 I=1,8
ISN 0184
                    DO 187 J=1,8
ISN 0185
                    DO 187 K=1,8
                187 \text{ U(I,J,K)} = \text{CT(J,I)*CTINV(I,K)}
ISN 0186
             C
             C
                    READ IN (NUMLTH) LENGTHS FOR THIS MEAN
              C
ISN 0187
                    KCOUNT = 0
ISN 0188
                190 READ (5,900) LENGTH
ISN 0189
                    KCOUNT = KCOUNT + 1
ISN 0190
                    WRITE (6,918) LENGTH
              C
              C
                    CALCULATION OF EXP(R*LENGTH)
              C
ISN 0191
                    DO 195 I=1,8
ISN 0192
                    DO 195 J=1,8
ISN 0193
                195 CR(I,J) = 0.0
ISN 0194
                    DO 200 K=1.8
ISN 0195
                    FACTOR = CDEXP(THETA(K)*LENGTH)
ISN 0196
                    DO 200 I=1,8
ISN 0197
                    DO 200 J=1,8
ISN 0198
                200 CR(I,J) = CR(I,J) + U(K,I,J)*FACTOR
ISN 0199
                    WRITE (6,985)
ISN 0200
                    WRITE (6,964) ((CR(I,J),J=1,8),I=1,8)
              C
                    CALCULATION OF EXP(R*LENGTH) USING H. G. SUBROUTINE
              C
ISN 0201
                    CALL EXMATR(R, T, LENGTH, 8, CORR, CONST, SDEV)
ISN 0202
                    WRITE (6,986)
ISN 0203
                    WRITE (6,975) ((T(I,J), J=1,8),I=1,8)
              C
              C
                    CALCULATION OF CONSTANTS MATRIX
ISN 0204
                209 DO 210 I=1.4
                    DO 210 J=1.4
ISN 0205
ISN 0206
                    REAL = CR(I,J)
ISN 0207
                    E11(I,J) = REAL
ISN 0208
                    REAL = CR(I, J+4)
ISN 0209
                    E12(I,J) = REAL
ISN 0210
                    CONST(I+4,J) = 0.0
                210 CONST(I+4,J+4) = 0.0
ISN 0211
ISN 0212
                    DO 215 I=5,8
                215 CONST (I,I) = 1.0
ISN 0213
ISN 0214
                    CALL MATINV (E11,4,82,0,DETERM,4)
ISN 0215
                    WRITE (6,946) DETERM
                    WRITE (6,964) ((E11(I,J),J=1,4),I=1,4)
ISN 0216
                    DO 220 I=1,4
ISN 0217
ISN 0218
                    DO 220 J=1,4
ISN 0219
                220 CUNST (I,J) = E11(I,J)
                    CALL CMTMLT (E11,4,4,E12,4,4,D)
ISN 0220
ISN 0221
                    DO 225 I=1,4
ISN 0222
                    DO 225 J=1,4
                225 CONST (I,J+4) = -D(I,J)
ISN 0223
ISN 0224
                    WRITE (6,990)
                    WRITE (6,965) ((CONST(I,J),J=1,8),I=1,8)
ISN 0225
             C
                    CALCULATION OF MATRICES Z'S AND W'S
              C
              C
ISN 0226
                    DO 240 I=1,8
ISN 0227
                    DO 240 J=1,8
                    DO 240 K=1,8
ISN 0228
ISN 0229
                    Z(I,J,K) = 0.0
                    DO 240 L=1,8
ISN 0230
                240 Z(1,J,K) = Z(1,J,K) + U(1,J,L)*CONST(L,K)
ISN 0231
```

```
DO 275 N1=1,8
ISN 0232
                    DO 270 J=1,8
ISN 0233
                    DU 250 I=1,4
ISN 0234
                250 W(N1, I, J) = Z(N1, I, J)
ISN 0235
                    DO 255 I=5,8
ISN 0236
                255 \text{ W(N1,I+2,J)} = \text{Z(N1,I,J)}
ISN 0237
                    W(N1,5,J) = 0.0
ISN 0238
                    W(N1,6,J) = 0.0
ISN 0239
ISN 0240
                    DO 260 L=1,4
                    W(N1,5,J) = W(N1,5,J) + GAM5(L)*Z(N1,L,J)
ISN 0241
                260 \text{ W(N1,6,J)} = \text{W(N1,6,J)} + \text{GAM6(L)}*Z(N1,L,J)
ISN 0242
                    DO 265 L=5,8
ISN 0243
                    W(N1,5,J) = W(N1,5,J) + GAM5(L+2)*Z(N1,L,J)
ISN 0244
                265 \text{ W(N1,6,J)} = \text{W(N1,6,J)} + \text{GAM6(L+2)*Z(N1,L,J)}
ISN 0245
                270 CONTINUE
ISN 0246
                275 CONTINUE
ISN 0247
                280 READ (5,930) X
ISN 0248
                    IF (X) 285,290,290
ISN 0249
             C
                    CALCULATION OF MEAN MATRIX
             C
ISN 0250
                290 DU 292 I=1,10
                    DU 292 J=1,8
ISN 0251
                    MEAN(I,J) = 0.0
ISN 0252
                    DG 292 K=1,8
ISN 0253
                292 MEAN(I,J) = MEAN(I,J) + (CDEXP(THETA(K)*X))*W(K,I,J)
ISN 0254
                    WRITE (6,935) LENGTH, X
ISN 0255
                    WRITE (6,937) M
ISN 0256
ISN 0257
                    DO 293 I=1,10
                    DO 293 J=1,8
ISN 0258
ISN 0259
                293 OMEAN(I,J) = MEAN(I,J)
                    WRITE (6,940)
ISN 0260
                    WRITE (6,965) ((OMEAN(I,J), J=1,8), I=1,10)
ISN 0261
                296 DO 297 I=1,10
ISN 0262
                   DO 297 J=1,8
ISN 0263
ISN 0264
                297 UMEAN(I,J) = (0.0,-1.0)*MEAN(I,J)
                    WRITE (6,967)
ISN 0265
ISN 0266
                    WRITE (6,965) ((OMEAN(I,J), J=1,8),I=1,10)
ISN 0267
                    GO TO 280
             C
                    CALCULATION OF SECOND FACTORIAL MOMENTS
             C
                    FIRST, CALCULATION OF X'S
ISN 0268
                285 CONTINUE
ISN 0269
                    STDEV = DSQRT(M2 + M - M*M)
ISN 0270
                    WRITE (6,840) M, STDEV
ISN 0271
                    DO 308 I = 1,10
ISN 0272
                    DU 308 J = 1.10
ISN 0273
               308 \text{ CUMP(I,J)} = P(I,J)
                   DO 310 IALPHA = 1,4
ISN 0274
ISN 0275
                    DO 310 IBETA = 1,8
ISN 0276
                    DU 310 IQ = 1,8
ISN 0277
                    DU 310 IR = 1,8
ISN 0278
                    DO 310 IL = 1,10
                    XTEMP1 = 0.0
ISN 0279
                    XTEMP2 = C.0
ISN 0280
ISN 0281
                    DO 305 IK = 1,10
ISN 0282
                    XTEMP1 = XTEMP1 + COMP(IL, IK) *W(IQ, IK, IALPHA)
ISN 0283
               305 XTEMP2 = XTEMP2 + COMP(IL, IK) *W(IR, IK, IBETA)
ISN 0284
               310 XX(IALPHA, IBETA, IQ, IR, IL) = XTEMP1*XTEMP2
ISN 0285
                    DO 320 L=1,4
ISA 0286
                    KAPPA5(L) = (M*P(L,5)*(1.0-M*P(6,6)) + M*P(L,6)*M*P(6,5))/DEN
ISN 0287
               320 KAPPA6(L) = (M*P(L,5)*M*P(5,6) + M*P(L,6)*(1.0-M*P(5,5)))/DEN
ISN 0288
                    DO 325 L = 5,8
ISN 0289
                    KAPPA5(L) = (M*P(L+2,5)*(1.0 - M*P(6,6)) + M*P(L+2,6)*M*P(6,5))/DE
                   1N
ISN 0290
               325 KAPPA6(L) = (M*P(L+2,5)*M*P(5,6) + M*P(L+2,6)*(1.0-M*P(5,5)))/DEN
                   CALCULATION OF Y'S
ISN 0291
                   RMM2 = -M2
```

```
DO 335 IALPHA = 1,4
ISN 0292
ISN 0293
                     DO 335 IBETA = 1,8
ISN 0294
                     DO 335 IQ = 1,8
ISN 0295
                     DO 335 IR = 1,8
                     DO 335 IL = 1,4
ISN 0296
ISN 0297
                     Y(IALPHA, IBETA, IQ, IR, IL) = (XX(IALPHA, IBETA, IQ, IR, IL) + KAPPA5(IL)
                    1*XX(IALPHA, IBETA, IQ, IR, 5) + KAPPA6(IL)*XX(IALPHA, IBETA, IQ, IR, 6))*
                    2(RMM2/MU(IL))
 ISN 0298
                335 Y(IALPHA, IBETA, IQ, IR, IL+4) = (XX(IALPHA, IBETA, IQ, IR, IL+6) + KAPPA5
                    1(IL + 4)*XX(IALPHA, IBETA, IQ, IR, 5) + KAPPA6(IL + 4)*XX(IALPHA, IBETA
                    2, IQ, IR, 6))*(RMM2/MU(IL+6))
                     CALCULATION OF INTEGRALS
                     DO 345 IALPHA = 1,4
 ISN 0299
 ISN 0300
                     DU 345 IBETA = 1,8
 ISN 0301
                     DU 336 IM = 1,8
 ISN 0302
                     INT(IM,8*(IALPHA-1) + IBETA) = 0.0
                 336
                     DO 345 IS = 1,8
 ISN 0303
 ISN 0304
                     DU 337 IM = 1,8
 ISN 0305
                 337 \text{ VTEMP(IM)} = 0.0
 ISN 0306
                     DO 340 IQ = 1.8
                     DU 340 IR = 1.8
 ISN 0307
                     FACTOR = (CDEXP((THETA(IQ) + THETA(IR) - THETA(IS))*LENGTH) - 1.0)
 ISN 0308
                    1/(THETA(IQ) + THETA(IR) - THETA(IS))
 ISN 0309
                     DU 340 IM = 1.8
 ISN 0310
                 340 VTEMP(IM) = VTEMP(IM) + Y(IALPHA, IBETA, IQ, IR, IM) *FACTOR
                     DO 344 IL = 1,8
 ISN 0311
                     DO 344 IM = 1,8
 ISN 0312
                 344 INT(IL, 8*(IALPHA-1) + IBETA) = INT(IL, 8*(IALPHA-1) + IBETA) +
 ISN 0313
                    1U(IS, IL, IM) *VTEMP(IM)
                 345 CONTINUE
 ISN 0314
               C
                     CALCULATION OF CONSTANTS MATRIX
               C
               C
 ISN 0315
                     DU 347 I = 1.4
                     DO 347 J = 1,32
 ISN 0316
                     INT2(1,J) = INT(1 + 4,J)
 ISN 0317
                     DU 350 I = 1,8
 ISN 0318
                     DO 350 J = 1,8
 ISN 0319
                 350 CR(I,J) = 0.0
 ISN 0320
                     DO 352 K = 1,8
 ISN 0321
                     FACTOR = CDEXP(THETA(K) *LENGTH)
 ISN 0322
 ISN 0323
                     DU 352 I = 1,8
                     DO 352 J = 1,8
 ISN 0324
                 352 CR(I,J) = CR(I,J) + U(K,I,J)*FACTOR
 ISN 0325
                     DO 355 I = 1,4
 ISN 0326
                     DO 355 J = 1.4
 ISN 0327
                     Ell(I,J) = CR(I,J)
 ISN 0328
 ISN 0329
                 355 E12(I,J) = CR(I,J+4)
                     CALL CMTMLT (E12,4,4,1NT2,4,32,1NT1)
 ISN 0330
                     CALL MATINV (E11,4,82,0,DETERM,4)
 ISN 0331
                     CALL CMTMLT ( E11, 4, 4, INT1, 4, 32, INT2)
 ISN 0332
                     DO 360 I = 1,4
 ISN 0333
                     DO 360 J = 1,32
 ISN 0334
                      SCONST(1+4,J) = 0.0
 ISN 0335
                 360 SCONST(I,J) = -INT2(I,J) - INT(I,J)
 ISN 0336
                     DO 362 I = 1,8
 ISN 0337
                     DO 362 J = 1,32
 ISN 0338
                 362 RSC(I,J) = SCONST(I,J)
 ISN 0339
                     WRITE (6, 1005)
 ISN 0340
                     WRITE (6,1010) ((RSC(I,J), J=1,32), I=1,8)
 ISN 0341
                     DO 365 I=1,8
 ISN 0342
                     DO 365 J=1,32
 ISN 0343
                 365 \text{ OCOV(I,J)} = (0.0,-1.0)*SCONST(I,J)
 ISN C344
                     WRITE (6,1020)
 ISN 0345
                     WRITE (6,1010) ((OCOV(I,J), J=1,32),I=1,8)
 ISN 0346
               C
               C
                     CALCULATIONS FOR ARBITRARY X
               C
ISN 0347
                 370 READ (5,930) X
```

```
IF (X) 450,375,375
ISN 0348
               375 DO 385 [ALPHA = 1,4
ISN 0349
                   DO 385 IBETA = 1.8
ISN 0350
                   DO 376 IM = 1,8
ISN 0351
               376 INT(IM, 8*(IALPHA-1) + IBETA) = 0.0
ISN 0352
                   DO 385 IS = 1,8
ISN 0353
                    DO 377 IM = 1,8
ISN 0354
               377 VTEMP(IM) = 0.0
ISN 0355
                    DO 380 IQ = 1,8
ISN 0356
                    FACTOR = (CDEXP((THETA(IQ) + THETA(IR) - THETA(IS))*X) - 1.0)/(THE
ISN 0357
ISN 0358
                   ITA(IQ) + THETA(IR) - THETA(IS))
                    DO 380 IM = 1,8
               380 VTEMP(IM) = VTEMP(IM) + Y(IALPHA, IBETA, IQ, IR, IM) *FACTOR
ISN 0359
ISN 0360
                   DO 384 IL = 1,8
ISN 0361
                    DO 384 IM = 1,8
                384 INT(IL,8*(IALPHA-1) + IBETA) = INT(IL,8*(IALPHA-1) + IBETA) +
ISN 0362
ISN 0363
                   1U(IS, IL, IM) *VTEMP(IM)
                385 CONTINUE
ISN 0364
                    DO 390 I = 1,4
ISN 0365
                    DO 390 J = 1,32
ISN 0366
                390 INT(I,J) = INT(I,J) + SCONST(I,J)
ISN 0367
                    DO 400 I = 1,8
ISN 0368
                    DO 400 J = 1,8
ISN 0369
                400 CR(I,J) = 0.0
ISN 0370
                    DO 405 K = 1.8
ISN 0371
                    FACTOR = CDEXP(THETA(K) *X)
ISN 0372
                    DU 405 I = 1,8
ISN 0373
                    DO 405 J = 1,8
ISN 0374
                405 \ CR(I,J) = CR(I,J) + U(K,I,J)*FACTOR
ISN 0375
                    CALL CMTMLT(CR,8,8,1NT,8,32,SMOP)
ISN 0376
                    WRITE (6,1015) X
ISN 0377
                    DO 410 I=1,8
ISN 0378
                    DO 410 J=1,32
ISN 0379
                410 \text{ OCOV}(I,J) = \text{SMOP}(I,J)
ISN 0380
                    WRITE (6,1010) ((OCOV(I,J), J=1,32), I=1,8)
ISN 0381
                    IF (LENGTH .NE. X) GO TO 414
ISN 0382
ISN 0384
                    DO 412 I=1,4
                    DO 412 J=1,32
ISN 0385
                412 SML(I,J) = OCOV(I+4,J)
ISN 0386
ISN 0387
                414 DO 415 I=1,8
                    DO 415 J=1,32
ISN 0388
ISN 0389
                415 \text{ OCOV}(I,J) = (0.0,-1.0)*SMOP(I,J)
                   WRITE (6,1025)
ISN 0390
ISN 0391
                    WRITE (6,1010) ((OCOV(I,J), J=1,32),I=1,8)
ISN 0392
                    GO TO 370
                    CALCULATION OF VARIANCES AND CORRELATIONS
ISN 0393
                450 DO 455 I=1,4
ISN 0394
                    DU 455 J=1,4
ISN 0395
                    VAR(I,J) = RSC(I,9*J - 8) + CONST(I,J)*(1.0-CONST(I,J))
ISN 0396
                455 VAR(I,J+4) = SML(5-I,37 - 9*J) + CONST(I,J+4)*(1.0-CONST(I,J+4))
ISN 0397
                    WRITE (6,925) ((VAR(I,J),J=1,8),I=1,4)
                    DO 470 I=1.4
ISN 0398
                    DO 460 IALPHA =1,4
ISN 0399
ISN 0400
                    IALP1 = IALPHA + 1
ISN 0401
                    DO 460 IBETA = IALP1,8
ISN 0402
                460 CORR(IALPHA, IBETA) = (RSC(I, 8*(IALPHA-1) + IBETA)
                   1 CONST(I, IALPHA) *CONST(I, IBETA)) / DSQRT(VAR(I, IALPHA) *VAR(I, IBETA))
ISN 0403
                    DO 465 IALPHA = 5,7
ISN 0404
                    IALP1 = IALPHA + 1
ISN 0405
                    DU 465 IBETA = IALP1,8
ISN 0406
                465 CORR(IALPHA, IBETA) = (SML(5-1,73 - 8*IALPHA - IBETA) -
                   1CONST(I, IALPHA) *CONST(I, IBETA))/DSQRT(VAR(I, IALPHA) *VAR(I, IBETA))
ISN 0407
                    DO 467 J=1,8
ISN 0408
                467 CORR(J,J) = 1.0
ISN 0409
                    DO 468 I1=2,8
ISN 0410
                    I1M1 = I1 - 1
ISN 0411
                    DO 468 J1 = 1, I1M1
ISN 0412
                468 CURR(11,J1) = CORR(J1,I1)
```

```
ISN 0413
                     WRITE (6,805) I
 ISN 0414
                     WRITE (6,810) (VAR(I,J), J=1,8)
 ISN 0415
                     DO 469 J1=1,8
 ISN 0416
                 469 SDEV(J1) = DSQRT(VAR([,J1))
 ISN 0417
                    WRITE (6,820)
 ISN 0418
                     WRITE (6,922) (CONST(I,J1), J1=1,8)
 ISN 0419
                     WRITE (6,922) (SDEV(J1), J1=1,8)
 ISN 0420
                     WRITE (6,815)
 ISN 0421
                     WRITE (6,922) ((CORR(11,J1),J1=1,8),I1=1,8)
                     IF (I .NE. 1) GO TO 470
 ISN 0422
 ISN 0424
                     DO 4690 I1 = 1.8
 ISN 0425
                     DU 4690 J1 = 1,8
                4690 CURR([1,J]) = CORR([1,J])*DSQRT(VAR([,[])*VAR([,J]))
 ISN 0426
 ISN 0427
                     WRITE (6,1030)
 ISN 0428
                     WRITE (6,922) ((CORR(II,J1), J1=1,8),I1=1,8)
                     SUM1 = 0.0
 ISN 0429
                     SUM2 = 0.0
 ISN C430
 ISN 0431
                     SUM3 = 0.0
 ISN 0432
                     DO 4692 I1 = 1,4
 ISN 0433
                     DO 4692 J1 = 1,4
 ISN 0434
                  SUM1 = SUM1 + CORR(II,JI)
 ISN 0435
                     SUM2 = SUM2 + CORR(11 + 4, J1 + 4)
 ISN 0436
ISN 0437
                4692 SUM3 = SUM3 + CORR(11, J1+4)
                     SUM = SUM1 + SUM2 + 2.0*SUM3
 ISN C438
                     SR = 0.0
 ISN 0439
                     ST = 0.0
 ISN 0440
                     DO 4694 J1 = 1,4
 ISN 0441
                     ST = ST + CONST(I,J1)
 ISN 0442
                4694 SR = SR + CUNST(I, J1 + 4)
 ISN 0443
                     SP = SR + ST
 ISN 0444
                     SUM1 = DSQRT(SUM1)
 ISN 0445
                     SUM2 = DSQRT(SUM2)
 ISN 0446
                     SUM = DSQRT(SUM)
 ISN 0447
                     WRITE (6,1040) LENGTH, M, STDEV
 ISN 0448
                     WRITE (6,1035) I, SK, SUM2, ST, SUM1, SP, SUM
 ISN 0449
                 470 CONTINUE
 ISN 0450
                     IF (KCOUNT .EQ. NUMLTH) GO TO 130
 ISN 0452
                     GU TO 190
                 500 STOP
 ISN 0453
 ISN 0454
                 8C5 FORMAT (////.25x.'VARIANCES AND CORRELATIONS FOR PARTICLES WITH IN
                    lITIAL DIRECTION', 13)
 ISN 0455
                 810 FURMAT (/,25x, VARIANCES FOR PARTICLES EMERGING IN DIRECTIONS 1-4
                   1 AND 7-10',/,5X,8D14.7,/)
                 815 FORMAT (/,25x, 'CORRELATION MATRIX',/)
 ISN 0456
                 820 FORMAT (26x, MEANS AND STANDARD DEVIATIONS FOR PARTICLES WITH THIS
 ISN 0457
                    1 INITIAL DIRECTION, ',/,26x, 'EMERGENT DIRECTIONS ARE 1-4 AND 7-10,
                    2WITH MEANS DIRECTLY ABOVE THE STANDARD DEVIATIONS',/)
 ISN 0458
                 835 FORMAT (1HO, 4CX, 'RAYLEIGH SCATTERING',/)
                 837 FORMAT (1HO, 40X, 'ISOTROPIC SCATTERING',/)
 ISN 0459
                 840 FORMAT (1HO,5X, MEAN NUMBER OF PARTICLES PRODUCED PER COLLISION IS
 ISN 0460
                    1',F10.5, 'STANDARD DEVIATION IS',F10.5,/)
 ISN 0461
                 880 FORMAT (10X, 2F10.8, 13)
                 900 FURMAT (10X,5F10.8)
 ISN 0462
                 902 FORMAT (13)
 ISN 0463
                 905 FORMAT (1H1,40X, 'MATRIX OF PROBABILITIES P(I,J)')
 ISN 0464
 ISN 0465
                 908 FORMAT (40X, G16.4)
                 910 FURMAT (10X, 10F12.8)
 ISN 0466
                 915 FORMAT (40X, MATRIX R')
 ISN 0467
                918 FORMAT (40X, 'LENGTH IS', F10.5)
 ISN 0468
                 920 FORMAT (40X, 'CHECK MATRIX')
 ISN 0469
 ISN 0470
                 922 FORMAT (2X,8F16.7)
925 FORMAT (10X,8D14.7)
 ISN 0471
                 930 FURMAT (F8.4)
 ISN 0472
                 935 FORMAT (1H1,10x, 'MEAN MATRIX FOR TOTAL LENGTH = 1, F5.2, WITH PARTI
 ISN 0473
                   ICLE AT POSITION X = 1, F5.2/)
                 937 FORMAT (10x, MEAN NUMBER OF PARTICLES PRODUCED PER COLLISSION IS',
 ISN 0474
                   1F8.4,/)
                 940 FORMAT (10x, 'ROW I REPRESENTS PARTICLE PRESENTLY TRAVELLING IN 1TH
 ISN 0475
                    1 DIRECTION. COLUMN J REPRESENTS PARTICLE EMERGING IN DIRECTION J'
                    2/1
                945 FURMAT (20x, 'NO. UF ITERATIONS =', 13, ' TIME(MS) =', F8.0)
ISN 0476
```

ISN	0477	946 FORMAT (4CX, DETERMINANT IS', 2D16.7,/)
	0478	950 FORMAT (40X, 'RETURNED MATRIX WITH EIGENVALUES'/)
ISN	0479	955 FORMAT (40X, 'THETAS')
ISN	0480	960 FURMAT (40X, EIGENVECTOR COLUMN MATRIX')
ISN	0481	964 FORMAT (2X,8D16.7/2X,8D16.7,/)
ISN	0482	965 FORMAT (2X.8D16.7./)
ISN	0483	967 FORMAT (1HO, 10X, 'IMAGINARY PART OF MEAN MATRIX. SHOULD BE ZERO'/)
ISN	0484	970 FORMAT (40X, INVERSE MATRIX OF EIGENVECTORS'/)
ISN	0485	975 FORMAT (2X,8F16.7,/)
ISN	0486	985 FURMAT (40X, 'EXP(R*LENGTH')
ISN	0487	986 FORMAT (40x, 'EXP(R*LENGTH) USING H. G. SUBROUTINE'/)
ISN	0488	990 FORMAT (40X, 'CONSTANTS MATRIX'/)
ISN	0489	1005 FURMAT (1H1,5X, CONSTANT MATRIX FOR SECOND FACTORIAL MOMENTS. PAR
		ITICLE AT O, I-TH ROW GIVES INITIAL DIRECTION 1-4, 7-10.',/5X,'(AL
		2PHA, BETA)-TH MOMENT IN COL. 8(ALPHA-1) + BETA, ALPHA = 1 TO 4 AND
		3BETA = 1 TO 4 AND (7 TO 10).')
ISN	0490	1010 FURMAT (4(2X,8D16.7/),/)
	0491	1015 FORMAT (10X, 'SECOND MOMENT OUTPUT, X = ',F8.4/)
ISN	0492	1020 FURMAT (1H0,20X, 'IMAGINARY PART OF CONSTANTS MATRIX. SHOULD BE ZE
		1RO.',/)
ISN	0493	1025 FORMAT (//,20X,'IMAGINARY PART OF SECOND FACTORIAL MOMENT OUTPUT.
		1 SHOULD BE ZERO.',//)
ISN	0494	1030 FORMAT (//,20x, VARIANCE-COVARIANCE MATRIX FOR PARTICLE INCIDENT A
		1T X = 0 TRAVELLING IN DIRECTION 1',//)
ISN	0495	1035 FORMAT (//, 20X, FOR PARTICLE AT X = 0 WITH INITIAL DIRECTION', 13,/
		1,9X, THE MEAN NUMBER OF PARTICLES REFLECTED IS',12X,F16.7, WITH S
		2TANDARD DEVIATION', F16.7, /, 9X, 'THE MEAN NUMBER OF PARTICLES TRANSM
		SITTED IS',10X,F16.7, WITH STANDARD DEVIATION',F16.7,/,9X, THE MEA
		4N OF THE TOTAL NUMBER OF PARTICLES PRODUCED IS ', F16.7, ' WITH STAND
		5ARD DEVIATION',F16.7,//)
ISN	0496	1040 FURMAT(/,20X, THE LENGTH OF THE SLAB IS',F10.4,/,20X, THE MEAN NUM
		1BER OF PARTICLES PRODUCED PER COLLISION IS',F10.4, WITH STANDARD
1.04	0107	2DEVIATION',F10.4)
121	0497	END

## ACKNOWLEDGEMENT

We are indebted to J. E. Moyal and Harold Greenspan for a number of valuable discussions and suggestions in connection with this work.

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